DISSERTATION

NUMERICAL SIMULATION OF GENERAL HYDRODYNAMIC DISPERSION IN POROUS MEDIUM

Submitted by

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In partial fulfillment of the requirements

for the Degree of Doctor of Philosophy

Colorado State University

Fort Collins, Colorado

August, 1971

CED71-72MN4

ABSTRACT OF DISSERTATION

NUMERICAL SIMULATION OF GENERAL HYDRODYNAMIC DISPERSION IN POROUS MEDIUM

A general two-dimensional equation of dispersion in a porous medium is presented. The second order linear partial differential equation describing the transient concentration distribution has mixed partial derivatives which is the result of treating the dispersion coefficients as second order symmetric tensors.

Using the principles of calculus of variations a "functional" is developed for the dispersion equation that has mixed partial derivatives. The two-dimensional region is divided into triangular finite elements of arbitrary size and shape. The concentration is assumed to vary linearly over each triangular finite element. Minimization of the functional in combination with the finite element method leads to a system of simultaneous, first order, linear, ordinary differential equations. The matrix differential equation is numerically integrated using the fourth order Runge-Kutta and Adams-Moulton multistep predictor-corrector methods.

Before proceeding with the use of the new functional, solutions were obtained for the dispersion equation with mixed partial derivatives in a rotated coordinate system. The numerical solutions using the new functional for one- and two-dimensional problems compared favourably with the available analytic solutions and the results obtained by finite element method that use a different functional. It was shown that the new funçtional can handle different ratios of lateral to longitudinal dispersion.

A general stability criteria for the resulting matrix equation is developed. Stability dependent on the data is discussed in detail with examples. A brief description of the numerical instability is also given.

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TO MY FAMILY

ACKNOWLEDGEMENTS

The author wishes to thank his advisor, Prof. R. A. Longenbaugh, for his encouragement, guidance and constructive comments. Thanks are extended to Dr. D. K. Sunada for his advice and ideas during the author's graduate study. The help and encouragement of Dr. D. B. McWhorter and Dr. A. B. Farnell are gratefully acknowledged.

The advice of Dr. E. A. Breitenbach, Dr. H. J. Morel-Seytoux and Dr. A. T. Corey is sincerely appreciated.

Sincere thanks are extended to Project 110 of the Colorado State University Experiment Station for providing the Graduate Research Assistantship. The funds provided by the University to cover computer costs is gratefully acknowledged.

Thanks are due to Miss Lyn Koch for typing the rough drafts. Final typing and reproduction were done by Type-Ink.

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CHAPTER I

INTRODUCTION

The ever increasing population of the world requires additional sources of freshwater for purposes of irrigation, industry and domestic supply. Freshwater from underground aquifers is one of the major sources available. The required quantity of this abundant supply with suitable quality properties is an important aspect to be considered in the water resources planning of many regions of the world. Ground water quality change is due to many factors, some of which are due to salt-water intrusion in coastal aquifers, underground waste disposal, recharge of surface water into underground storage and pollution of ground water by infiltration from streams and rivers. An understanding of the mechanics of ground water flow and the phenomenon of miscible fluid displacement is essential to make an estimate of the quantity and quality of the available ground water.

1.1 Description of the problem:

The problem of increasing contamination is becoming more and more important with regard to the ground water industry. Changes in ground water quality can be described by the hydrodynamic dispersion equation with coefficients depending on the flow and porous medium as well as on the solvent and solute. Dispersion is an anisotropic process and the dispersion coefficients should be treated as second order, symmetric tensors. In a two-dimensional flow field, this leads to a non-symmetrical, linear partial differential equation of second order that has mixed partial derivatives representing the transient concentration distribution.

1.2 Objectives:

A review of the literature on dispersion in ground water and advances in computer methods indicated it might be possible to effectively simulate the dispersion process by numerical techniques. Investigators have used both finite difference and finite element methods for numerically solving the dispersion equation. The finite element method is further evaluated in this study.

Finite element method: The concept of the "finite element" approach can be used for problems in which the exact solution is defined as that which minimizes some integral of the unknown function or of its derivatives. This integral is known as the "functional" of the problem (Zienkiewicz and Cheung, 1967). If the unknown function is defined throughout the region, element by element, in terms of the values of the function at the node points of the elements, then the minimization of the functional will result in a series of ordinary differential equations equal in number to that of the unknown values of the function at the nodes.

With this background in mind the following objectives were pursued:

1. Develop a functional to solve by finite element method the general hydrodynamic dispersion equation in two dimensions having mixed partial derivatives.
2. Consider the lateral dispersion and molecular diffusion in computing the tensor of the dispersion coefficients.
3. Evaluate the stability and convergence criteria of the numerical simulator.
4. Compare the results obtained by the finite element method with that of the available analytic solutions of the dispersion equation for simple cases.
5. Compare the results with other finite element solutions that use different functionals.

CHAPTER II

REVIEW OF LITERATURE

Many investigators have studied the problem of hydrodynamic dispersion in porous media. These investigations may be divided into the following categories:

1. Theoretical developments;
2. Analytical results for simple cases;
3. Experimental work to test the validity and limitations of the theoretical results and to obtain the magnitude of the dispersion coefficients;
4. Numerical approximations for both the simple cases and for more complex geometries and flow situations.

Most of the works assume no interaction between fluid and porous media, and therefore, the miscible displacement is considered stable. As water with dissolved salts moves through the porous medium, the salts in the water will interact with the earth materials and thus the ground water quality is controlled to some extent by this hydrochemical phenomenon. Guymon (1970) gives a short review of the research on hydrochemical phenomena related to ground water quality.

2.1 Theoretical developments:

In general one is concerned with the variation in concentration created by both dispersion and diffusion. Diffusion is a direct result of thermal motion of the individual fluid molecules and takes place under the influence of a concentration gradient. Dispersion in porous media is a mechanical or convective mixing process which is the result of individual fluid particles traveling at variable velocities through irregular shaped pores and along tortuous microscopic pathlines (Reddell, 1969). That is, dispersion is the result of convective mixing on a microscopic scale; not of a concentration gradient.

Investigators proposed different relationships for the diffusion and dispersion coefficients. Taylor (1953, 1954) used a bundle of capillaries and investigated the displacement of a fluid from a straight capillary tube of radius, r, by another fluid miscible with the first. He found that the tracer was dispersed relative to a plane moving with velocity, V, as in Fick's first law, but with a diffusion coefficient:

$$D = \frac{r^2 V^2}{48 D_d} \qquad (2\text{-}1)$$

where D_d = molecular diffusion coefficient. This diffusion coefficient D (Eq. 2-1) has not been used in solving the dispersion equation.

Scheidegger (1961) suggested that the dispersion coefficient:

$$D_{ij} = \epsilon_{ijmn} \frac{V_m V_n}{V} \qquad (2\text{-}2)$$

where: ϵ_{ijmn} is the coefficient of dispersivity, which is a porous medium property,

$\frac{V_m V_n}{V}$ is a tensor which represents the linear influence of velocity,

and V_m, V_n are the components of velocity in the m and n directions respectively.

He concluded that the coefficient of dispersivity was a fourth rank tensor with 81 components; but due to certain symmetry properties, contains only 36 independent components in the general case of an anisotropic medium. In isotropic media there are only two dispersivity coefficients. From the results of de Josselin de Jong (1958), Bear (1961a) developed an expression for the dispersion coefficients, D_{ij}, and implied that it was a second-rank symmetrical tensor linear in the components of the velocity.

Bachmat and Bear (1964) present the following general equation of dispersion in homogeneous, isotropic porous media, which results from the mass balance approach:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left[D_{ij} \frac{\partial C}{\partial x_j} - u_i C \right] \tag{2-3}$$

where C = Concentration of dispersing mass,

t = time,

u_i = seepage velocity in the i-direction,

x_j = Cartesian coordinates,

D_{ij} = components of the coefficient of dispersion, a second-order symmetric tensor, which does not include molecular diffusion,

and i, j = index coordinates.

They also express the dispersion equation in curvilinear coordinates consisting of stream lines, ψ, and equipotentials, Φ. The equation in ψ - Φ coordinate system has the advantage of having only one convective term.

Reddell and Sunada (1970) and De Wiest (1969, Chapter 4) present a form of Eq. 2-3 which included the effects of molecular diffusion. The equation is:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left[D^*_{ij} \frac{\partial C}{\partial x_j} - u_i C \right] \qquad (2\text{-}4)$$

where
$$D^*_{ij} = D_{ij} + D_d\, T_{ij} \qquad (2\text{-}5)$$

In Eq. 2-5, D^*_{ij} = hydrodynamic dispersion coefficients independent of the concentration C (second order tensor),

D_d = molecular diffusion coefficient (scalar),

T_{ij} = porous medium "tortuosity" (dimensionless and second order tensor),

and other variables are as defined earlier. Eq. 2-4 is a linear, non-symmetrical partial differential equation. The non-symmetry is due to the convective term $\frac{\partial}{\partial x_i}\left(u_i C\right)$.

2.2 Analytical results:

The analogy between heat conduction and diffusion has been used to develop analytic solutions for a few simple cases. As the diffusion equation is similar to the heat flow equation, the solutions are also similar. Carslaw and Jaegar (1959) and Crank (1956) are two of the good references for analytical solutions of heat conduction and diffusion problems respectively. An example of an analytical solution for the dispersion equation is given below for a problem having steady, uniform and one-dimensional flow.

Consider a semi-infinite column $(x > 0)$ of homogeneous and isotropic porous media with initial and boundary conditions as shown in Fig. 2-1. Only longitudinal dispersion will occur and Eq. 2-3 reduces to:

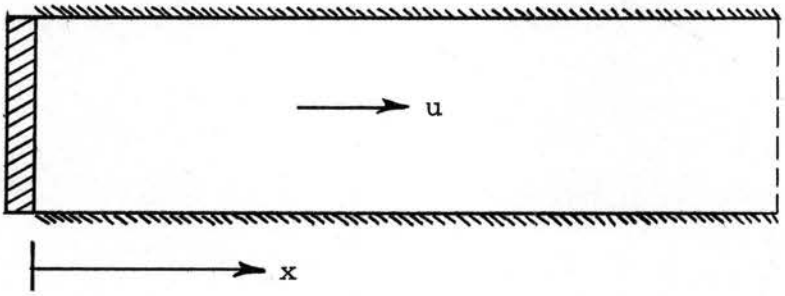
$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} \qquad (2\text{-}6)$$

where D_L is the longitudinal dispersion coefficient.

Using Laplace transform, Ogata and Banks (1961) obtained the solution for Eq. 2-6 as:

$$\frac{C}{C_o} = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x-ut}{2\sqrt{D_L t}}\right) + \exp\left(\frac{ux}{D_L}\right) \operatorname{erfc}\left(\frac{x+ut}{2\sqrt{D_L t}}\right)\right] \qquad (2\text{-}7)$$

where $\operatorname{erfc}(w) = 1 - \operatorname{erf}(w)$.



I.C.: $C(x, 0) = 0$ for $x \geq 0$

B.C.: $C(0, t) = C_o$ for $t \geq 0$

$C(\alpha, t) = 0$ for $t \geq 0$

Fig. 2-1 Semi-infinite column of porous medium.

This analytic solution enables us to compare the numerical solutions for similar problems.

When $D_L < 0.002$ ux, the second term in Eq. 2-7 may be neglected and the maximum error will be less than three percent.

2.3 <u>Experimental work</u>:

In most of the cases, the main purpose of the experiments have been to verify the theories proposed and to establish relationships to calculate the dispersion coefficients from media and fluid properties.

Scheidegger's (1961) work indicated that for homogeneous and isotropic media, the dispersion tensor reduces to two independent terms: (1) D_L, the longitudinal dispersion coefficient, and (2) D_T, the lateral dispersion coefficient.

The Reynold's number has been used as a parameter to correlate the dispersion coefficients. Ebach and White (1958) postulated from their experiments that for Reynold's number $R_n < 100$:

$$\frac{D_L}{\nu} = \alpha_1 \left(\frac{Vd^*}{\nu}\right)^{\beta_1} \tag{2-8}$$

where V = seepage velocity of fluid,

d^* = particle size of the porous media,

and ν = kinematic viscosity of the fluid.

α_1 and β_1 are experimentally determined coefficients, dependent on the porous medium and flow regime respectively. Ebach and White (1958) found $\alpha_1 = 1.92$ and $\beta_1 = 1.06$. Harleman and Rumer (1963) found $\alpha_1 = 0.66$ and $\beta_1 = 1.2$. Hoopes and Harleman (1965) found $\alpha_1 = 1.7$ and $\beta_1 = 1.2$. The variations in these values may be attributed to the experimental techniques for measuring concentration.

Harleman, et al (1963) correlated longitudinal dispersion with permeability:

$$\frac{D_L}{\nu} = \alpha_2 \left(\frac{V\sqrt{K}}{\nu}\right)^{\beta_2} \tag{2-9}$$

where K is the unit of permeability with dimensions L^2 and they found $\alpha_2 = 54$ for spheres and 88 for sand with $\beta_2 = 1.2$ for both media.

Using a similar approach to determine the lateral dispersion coefficient D_T, an expression of the form:

$$\frac{D_T}{\nu} = \alpha_3 \left(\frac{V d^*}{\nu}\right)^{\beta_3} \tag{2-10}$$

was used by Harleman and Rumer (1963) and they found $\alpha_3 = 0.036$ and $\beta_3 = 0.7$.

Bear (1961b) concluded from his experiments that the dispersion coefficient, D_s, in the s-direction can be expressed in the form:

$$D_s = d|V_s| \tag{2-11}$$

where d is a constant depending on the media characteristics and V_s is the seepage velocity in the s-direction. Guymon (1970) used this relationship in his work. Eq. 2-11 treats the dispersion coefficient as an isotropic quantity and thus excludes the mixed partial derivatives from the partial differential equation describing the concentration distribution.

Bruch (1970) conducted a series of two-dimensional dispersion experiments and verified some of the theoretical and numerical results. He treated the dispersion coefficient as an isotropic quantity, and included the lateral dispersion coefficient. The results demonstrated the need to consider the combined effect of longitudinal and lateral dispersion in the analysis.

2.4 Numerical approximations of ground water equations:

Need for a numerical approach: Most of the available analytical results are based on a set of assumptions which are to a certain extent at variance. These assumptions are made to simplify the complex mathematics involved in the problem and also because of lack of accurate data. The quantitative reliability of the results obtained from these analytical approaches depends on the degree of variance in the assumptions made. In the experimental work different types of physical models have been used either to verify or to improve upon the existing theories of dispersion in ground water flow and to determine the dispersion coefficients. However, these physical models do not exactly simulate the field conditions and it is understood that to date (1971) no laboratory techniques have been developed to exactly model the complex prototype situations. Because of these difficulties, many investigators are using numerical methods to obtain approximate solutions of the dispersion equation for complex, prototype problems. The development of high speed computers enhance such an approach.

Numerical methods have been used for solving both flow equations and dispersion equations. Solution of the flow equation is needed to compute the velocity components to be used for solving the dispersion equation. Investigators have used both the finite difference and finite element methods.

Finite difference method for solving the flow equation: Numerical finite difference methods have been very widely used for the case of immiscible fluid flow through porous media. Many of the reservoir simulation techniques were developed by the petroleum industry. Some work has been done in the area of ground water hydrology. Tyson and Weber (1964) have used computer simulation techniques to model ground water basins. The zone was divided into polygons and the unknown function was computed at a finite number of node points lying within the boundaries of the aquifer. They successfully evolved and tested a mathematical model of a ground water basin.

Bittinger, et. al. (1967) used the finite difference method for simulating a mathematical model for better aquifer management. They used rectangular grids for computing the head at the center of each grid. The resulting equations have a particularly simple symmetrical form. Brutsaert (1970) presented results on an immiscible fluid flow simulator. He used a fully implicit finite difference scheme and obtained satisfactory results for an unconfined well flow problem treated as a multiphase flow phenomenon.

Finite element method for solving the flow equation: This method was originally developed in the field of stress analysis. There have been some recent publications on the use of the finite element method for steady state and time dependent fluid flow and heat conduction problems. Neuman and Witherspoon (1970b) presented functionals based on variational principles for confined and unconfined flow of ground water.

Zienkiewicz and Cheung (1965) used this method for solving "field problems" which require the solution of a differential equation throughout a physical region or "field." Zienkiewicz, et. al. (1966) solved an anisotropic, steady state seepage problem. Taylor and Brown (1967) have used this method for steady state Darcy flow solutions with a free surface. Neuman and Witherspoon (1970a) analyzed steady state seepage with a free surface, using the finite element method and a new iterative approach to obtain rapid convergence. Their method can handle problems where the free surface is discontinuous and where portions of the free surface are vertical or near vertical.

Recently the U. S. Army Corps of Engineers (1970) used the finite element method to solve steady state potential flow problems.

For a regional ground water problem, they obtained good correlation between the observed potentiometric surface and the computed values of the hydraulic head. The results from the problem on axisymmetric radial flow to a well and that from the problem on steady state seepage from a ditch considering the effects of capillarity proved the versatility of the finite element method.

Wilson and Nickell (1966) applied the finite element method for transient heat conduction analysis of complex solids and concluded that this method possesses unique advantages as compared to other numerical approaches with respect to treating variable distribution of thermal properties, temperature and heat flux boundary conditions and solids of arbitrary geometric shape. They further said that the method provides an efficient digital computer approach for a large class of time dependent problems.

Javandel and Witherspoon (1968), Witherspoon, et. al. (1968), Javandel and Witherspoon (1969) have solved transient fluid flow in porous media using the finite element method. They claim that the generality of this method with respect to arbitrary boundary conditions and changes in rock properties provides a powerful new method of handling problems of fluid flow in complex systems. Very recently, France, et. al. (1971) solved by the finite element method the three-dimensional, steady state and transient seepage problems using the isoparametric concept. According to them, the technique of considering the time variant problem as a series of steady state solutions separated by a small time interval is ideally suited to the digital computer. They conclude that much work remains to be done in the field of finite element application to free surface problems in general.

Finite difference method for solving dispersion equation: Some work has been done on the use of the finite difference method for solving the hydrodynamic dispersion equation. Peaceman and Rachford (1962) used Darcy's law for flow and a dispersion equation in Cartesian coordinates for a two-dimensional case. After computing pressure distribution at each time step, the velocities are determined. Using these velocities, the new concentration distribution for the next time step may be computed from the dispersion equation. Garder, et. al. (1964) used the method of characteristics for treating combined transport and dispersion to improve the numerical solution of the problem solved by Peaceman and Rachford (1962). This method involves, in addition to the usual division of the two-dimensional space into rectangular grids, the use of a set of moving points. Each moving point has associated with it a concentration, which varies with time. This method prevents numerical dispersion although it involves more computer storage.

Shamir and Harleman (1967) used equipotentials and streamlines ($\Phi - \psi$) coordinates as the basis for the numerical scheme to solve the problems of dispersion in which the miscible fluids have the same density and viscosity. In this case, the velocity is everywhere tangential to the streamlines and the equation becomes one-dimensional in the convective term. In some of the problems in which the boundary conditions were constant at a concentration equal to C_o, the relative concentration C/C_o were greater than one $(C/C_o > 1.0)$ behind the advancing front. Shamir and Harleman (1967) developed and tested the numerical scheme for two-dimensional problems and presented an extension for three-dimensional problems.

Reddell (1969) used the finite difference method for the study of dispersion in ground water aquifers. He employed an implicit numerical technique to solve the flow equation for pesssure in an unsteady, non-uniform flow field with density and viscosity variations between the two fluids, and the method of characteristics with a tensor transformation to solve the convective dispersion equation. After solving for pressures in the flow equation, velocities were computed using Darcy's law and these velocities were used, after correcting for porosity of the medium, in solving for the concentration in the convective dispersion equation. Thus, the solution of the flow equation and the dispersion equation constitutes one time step. For the next time step, the new values of the concentrations obtained by solving the dispersion equation at the end of the previous time step are used in the flow equation to solve for pressures and the process repeated. This is known as a "leap frog" technique. A salt water intrusion problem in a coastal aquifer was modeled.

Pinder and Cooper, Jr. (1970) also used the method of characteristics and a simplified flow equation in conjunction with the iterative alternating direction implicit procedure for predicting the movement of the salt water front in coastal aquifers. The method used by Reddell (1969) is more sophisticated than that of Pinder and Cooper, Jr. (1970).

Finite element method for solving dispersion equation: More recently, Guymon (1970) used the finite element method for predicting the motion of dissolved constituents in ground water aquifers in a two-dimensional, steady flow field. The dispersion coefficients were not treated as tensors, Eq. 2-11. Only the longitudinal dispersion coefficient was considered and he neglected the lateral dispersion and molecular diffusion. Velocities and saturated thicknesses are considered as given information. His model deals with only physical and mechanical aspects of the motion of the dissolved constituents in ground water flow. The objectives of his research were to provide the basic mathematical and conceptual frame work to model a complex multi-aquifer regional ground water basin in order to predict with a reasonable degree of precision the spatial and time varying concentrations of selected dissolved salt species pumped from a well.

Though Guymon (1970) was the first to use the finite element method to solve the dispersion equation, some of his assumptions could be avoided. For example, the dispersion coefficient may be treated as an anisotropic quantity which will lead to a partial differential equation having mixed partial derivatives. In addition, the lateral dispersion and molecular diffusion may be included as a tensor in the dispersion coefficients.

2.5 Further needs for finite element method for solving dispersion equation:

In solving the convective dispersion equation using the finite difference methods, some difficulties have been reported. Subsequent testing of the method adopted by Peaceman and Rachford (1962) has shown that for multi-dimensional displacement, their method involved a numerical dispersion of the same order of magnitude as the physical dispersion. Numerical dispersion is an effective dispersion caused by the finite difference approximation and produces dispersion even when the dispersion coefficients are set equal to zero. Hoopes and Harleman (1965) used an explicit finite difference method, and in this, the size of the grid spacing and time increment were restricted for the explicit scheme because of stability criterion. This presented some problems because of large amounts of required computer time. The method of characteristics used by Reddell (1969) involves the use of "moving points", in addition to stationary finite difference grids and this requires extensive computer storage and execution time. It is easier to handle the irregular boundary shapes by the finite element method.

To solve large problems, the required computer storage and time become important factors. From his experience, Guymon (1970) concluded that the computer program based on the finite element method is more accurate and requires smaller computer storage and execution times than programs which are based on finite difference methods for solving the convective dispersion equation; however, he has not presented any evidence to support this statement. The finite element method is applicable to irregular basin configurations that are divided into any selected number of triangular elements of arbitrary size and shape. This method is particularly suited to basins having irregular boundaries, i.e., it provides a complete geometrical flexibility.

If the dispersion coefficient in porous media is treated as a second rank tensor, the resulting second order linear partial differential equation has mixed partial derivatives. The dispersion coefficients as given by Eq. 2-5 are linear functions of the velocity components and molecular diffusion. The proposed scheme is an improvement over that of Guymon (1970) in that the basic differential equation is more general as it includes the mixed partial derivatives. Also, the dispersion coefficients consist of longitudinal and lateral dispersion and molecular diffusion.

CHAPTER III

MATHEMATICAL MODEL AND NUMERICAL SIMULATOR

In this chapter, the general form of the hydrodynamic dispersion equation is presented with the auxiliary equations. A functional is developed utilizing the variational principles for the two-dimensional dispersion equation and an extension is suggested for solving the ground water flow equation. A numerical simulator is developed using the finite element technique.

3.1 Methods of approach:

The finite element technique is an approximate method of analysis similar to the finite difference method. The finite element technique, on the other hand, uses an associated functional instead of solving directly the differential equation. The approach to the problem by the finite element technique may be divided as follows:

1) Derive the appropriate differential equation and specify the necessary boundary conditions;
2) Develop the associated functional and prove the equivalence between the functional and the differential equation with suitable boundary conditions;
3) Divide the region into triangles (finite elements) of arbitrary size and shape;

4) Minimize the functional for each triangular element using variational principles;

5) Group the resulting equations from all elements;

6) Modify for constant concentration boundary conditions;

7) Solve the system of equations;

8) Develop the stability criteria for the system of equations.

3.2 Mathematical model:

Dispersion equation: It is generally accepted that the dispersion equation in Cartesian coordinate system is Eq. 2-3, which is obtained from the principles of conservation of mass. The equation for the conservation of mass of the dispersing material in an elementary control volume is obtained by equating the time rate of accumulation of mass inside the volume to the net influx of mass through the boundaries of the element. The net influx is made up of convective terms and terms involving dispersion. The modified form of the dispersion coefficients by Reddell and Sunada (1970) are presented in Eq. 2-5, which includes the longitudinal and lateral dispersion and molecular diffusion.

Guymon (1970) and Guymon, et. al. (1970) treated the dispersion coefficients as being isotropic, thus reducing Eq. 2-3 to one without mixed partial derivatives. They further neglected the lateral dispersion and molecular diffusion. The dispersion coefficient given by Eq. 2-5 is an anisotropic quantity and thus should be treated as a second rank tensor. Eq. 2-4 can be written after dropping the superscripts (in two-dimensional Cartesian coordinates) as:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y} + D_{yx}\frac{\partial C}{\partial x}\right) \qquad (3\text{-}1)$$

where u = seepage velocity in the x-direction,

v = seepage velocity in the y-direction,

and the dispersion coefficients D_{xx}, D_{yy}, D_{xy}, and D_{yx} are obtained from Eq. 2-5 as follows:

$$D_{xx} = D_L \frac{u^2}{V^2} + D_T \frac{v^2}{V^2} + D_d T$$

$$D_{yy} = D_T \frac{u^2}{V^2} + D_L \frac{v^2}{V^2} + D_d T \qquad (3\text{-}2)$$

and $$D_{xy} = D_{yx} = (D_L - D_T)\frac{uv}{V^2} \quad .$$

In Eq. 3-2, the seepage velocity V is defined as Darcy's velocity divided by the porosity of the medium. Other variables in Eqs. 3-1 and 3-2 are as defined earlier.

Because of the symmetric nature of the dispersion coefficients, $D_{xy} = D_{yx}$, Eq. 3-1 may be written as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_{xx}\frac{\partial^2 C}{\partial x^2} + 2D_{xy}\frac{\partial^2 C}{\partial x \partial y} + D_{yy}\frac{\partial^2 C}{\partial y^2} \qquad (3\text{-}3)$$

Eq. 3-3 describes the transient concentration distribution in a two-dimensional case.

The types of boundary conditions to be considered to solve Eq. 3-3 by the finite element method are:

$$C = C_o(x, y) \text{ on a portion of the boundary for } t \geq 0\,, \tag{3-4}$$

$$\text{and } \frac{\partial C}{\partial n} = 0 \text{ for the remaining portion of the boundary for } t \geq 0, \tag{3-5}$$

where n represents the direction normal to the boundary. Eq. 3-4 is called a geometric or fixed boundary condition and Eq. 3-5 would be a natural or reflective boundary condition (Shamir and Harleman, 1967).

Dispersion equation in rotated coordinate system: It is possible to account for the mixed partial derivatives of Eq. 3-3 by rotating the coordinates through an angle θ. The transformed axes are orthogonal and denoted by $x'\,y'$. In this $x'\,y'$ coordinate system, Eq. 3-3 becomes:

$$\frac{\partial C}{\partial t} + u' \frac{\partial C}{\partial x'} + v' \frac{\partial C}{\partial y'} = D_{x'x'} \frac{\partial^2 C}{\partial x'^2} + D_{y'y'} \frac{\partial^2 C}{\partial y'^2} \tag{3-6}$$

$$\text{where} \quad \theta = \tfrac{1}{2} \tan^{-1} \left(\frac{2D_{xy}}{D_{xx} - D_{yy}} \right),$$

$$D_{x'x'} = D_{xx} \cos^2 \theta \quad 2D_{xy} \sin\theta \cos\theta + D_{yy} \sin^2 \theta,$$

$$D_{y'y'} = D_{xx} \sin^2 \theta - 2D_{xy} \sin\theta \cos\theta + D_{yy} \cos^2 \theta,$$

$$u' = (u \cos\theta + v \sin\theta),$$

and $$v' = -(u \sin\theta - v \cos\theta).$$

The proof for Eq. 3-6 is given in Appendix A. Though Eq. 3-6 includes the effect of the mixed partial derivatives, it has some limitations which will be explained in Chapter IV.

3.3 Variational principles and proof of equivalence:

> "There is an entire class of engineering problems which pose such questions as what is most...? Where is minimum...? or How can we best...? In this class of optimization problems, one finds a sub-class which is formulated in the language of variational calculus."
>
> (Schechter, 1967)

In many of these problems, the minimization of some integrated quantity (referred to usually as a "functional") and subject to some boundary conditions results in the exact solution of equations such as Eq. 3-3. This functional may represent a physically recognizable variable in some instances. It is then usually associated with concepts of energy or work. For many purposes, however, it is simply a mathematically defined entity (Zienkiewicz, 1967).

The finite element method of solving problems in ground water are usually based on variational principles. A variational principle is a complete representation of the problem in the sense that the initial and boundary conditions are part of the functional (Neuman and Witherspoon, 1970b). The basic approach is to replace the boundary value problem by an appropriate functional whose minimizing function is the solution to the problem. If C^* is the exact solution to the dispersion Eq. 3-3 and if $J(C)$ represents the functional for Eq. 3-3, then the variational principle states that the functional $J(C)$ should attain its minimum value at C^*. Among the family of functions we can find a particular C for which $J(C)$ holds the least value. Utilizing these basic concepts of the variational principles and the functional for the associated differential equation, the finite element method is used to solve the hydrodynamic dispersion equation in a two-dimensional case.

Many problems in science and engineering involving rates of change with respect to two or more independent variables, usually representing time, length or angle can be expressed as partial differential equation or a set of such equations. Special cases of the two-dimensional second order equation:

$$a \frac{\partial^2 w}{\partial x^2} + 2b \frac{\partial^2 w}{\partial x \, \partial y} + c \frac{\partial^2 w}{\partial y^2} + d \frac{\partial w}{\partial x} + e \frac{\partial w}{\partial y} + f w + g = 0 \qquad (3\text{-}7)$$

where a, b, c, d, e, f and g may be functions of x and y, and of the dependent variable w, occur more frequently than any other because they are often the mathematical form of one of the conservation principles. If it is assumed that the coefficients may be functions of x and y only, Eq. 3-7 becomes linear and is derivable from a variational problem of the form:

$$\delta \iint_R \left[\tfrac{1}{2}\left(a\, w_x^2 + 2b\, w_x w_y + c\, w_y^2 - f\, w^2\right) - g\, w\right] A\, dxdy = 0 \qquad (3\text{-}8)$$

where appropriate boundary conditions are prescribed (Hildebrand, 1965). In Eq. 3-8, $A = A(x, y)$ may be termed a reducing factor and δ denotes a small variation. Eq. 3-8 is to be integrated over the two-dimensional region R (Fig. 3-1).

In Eq. 3-3 the dispersion coefficients D_{xx}, D_{xy}, and D_{yy}, and the velocity components u and v are assumed to be functions of x and y only, and at any instant of time $\frac{\partial C}{\partial t}$ is considered as invariant at any particular point in space. By analogy with Eqs. 3-7 and 3-8, the variational problem for Eq. 3-3 may be written as:

$$\delta \iint_R \exp(\beta) \left\{ \tfrac{1}{2}\left[D_{xx}\left(\frac{\partial C}{\partial x}\right)^2 + 2\, D_{xy}\left(\frac{\partial C}{\partial x}\right)\left(\frac{\partial C}{\partial y}\right) + D_{yy}\left(\frac{\partial C}{\partial y}\right)^2 \right] + \left(\frac{\partial C}{\partial t}\right) C \right\} dx\, dy = 0 \qquad (3\text{-}9)$$

where $\exp(\beta)$ is the reducing factor and

$$\beta = -\left(\frac{ux + vy}{D_L + D_d T}\right) \qquad (3\text{-}10)$$

The proofs for the reducing factor $\exp(\beta)$ and for Eq. 3-10 are given in Appendix B. Eq. 3-9 is to be integrated over the two-dimensional region R (Fig. 3-1).

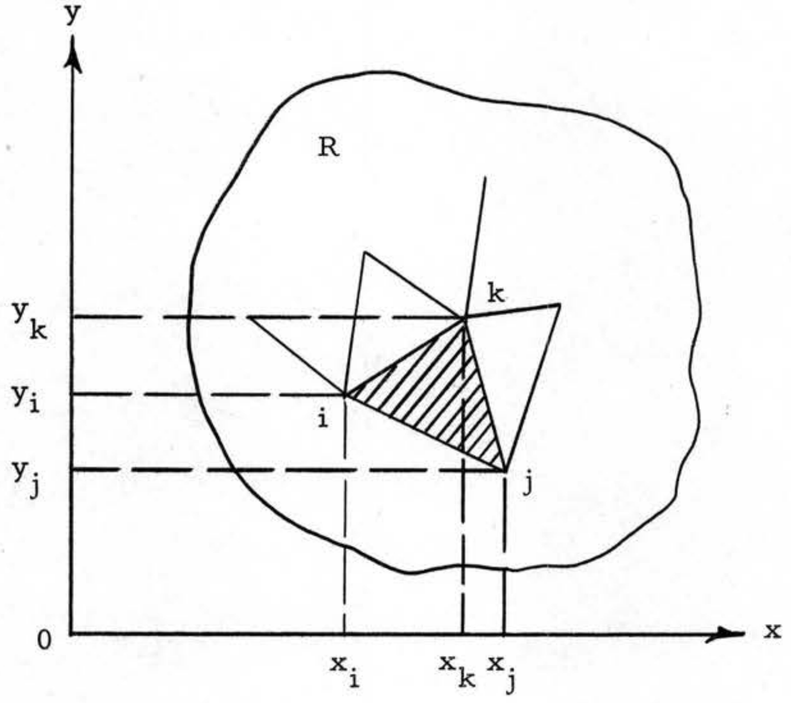


Fig. 3-1 Division of the two-dimensional region R into triangular finite elements.

The appropriate functional J for Eq. 3-3 is:

$$J = \iint_R \exp(\beta) \left\{ \tfrac{1}{2} \left[D_{xx} \left(\frac{\partial C}{\partial x}\right)^2 + 2\, D_{xy} \left(\frac{\partial C}{\partial x}\right)\left(\frac{\partial C}{\partial y}\right) + D_{yy} \left(\frac{\partial C}{\partial y}\right)^2 \right] + \left(\frac{\partial C}{\partial t}\right) C \right\} dx\, dy \tag{3-11}$$

where β is defined by Eq. 3-10. The proof that this functional is equivalent to the differential Eq. 3-3 and the boundary conditions (Eqs. 3-4 and 3-5) is shown in Appendix B.

Due to numerical difficulties in solving for the concentration C, elaborated upon by Guymon, et. al. (1970), a change of variable is introduced by the transformation:

$$\phi = C \exp(\beta/2) \tag{3-12}$$

where ϕ is the new dependent variable. Using this new variable ϕ, and assuming the dispersion coefficients and velocity components as constants, the original differential Eq. 3-3 is transformed as:

$$\frac{\partial \phi}{\partial t} + \left[\frac{D_{yy} u^2 + D_{xx} v^2 - 2 D_{xy} uv}{4(D_{xx} D_{yy} - D_{xy}^2)} \right] \phi = D_{xx} \frac{\partial^2 \phi}{\partial x^2} + 2\, D_{xy} \frac{\partial^2 \phi}{\partial x \partial y} + D_{yy} \frac{\partial^2 \phi}{\partial y^2} \tag{3-13}$$

To avoid zero in the denominator of the coefficient of ϕ on the left hand side of Eq. 3-13, the relationships for the dispersion coefficients, Eq. 3-2, may be used and Eq. 3-13 becomes:

$$\frac{\partial\phi}{\partial t} + \left[\frac{u^2 + v^2}{4(D_L + D_d T} \right] \phi = D_{xx} \frac{\partial^2\phi}{\partial x^2} + 2D_{xy} \frac{\partial^2\phi}{\partial x\,\partial y} + D_{yy} \frac{\partial^2\phi}{\partial y^2} \tag{3-13a}$$

The boundary conditions given by Eqs. 3-4 and 3-5 respectively are transformed as:

$$\phi = \phi_o(x, y) = C_o(x, y) \exp(\beta/2) \tag{3-14}$$

on a portion of the boundary for $t \geq 0$,

and
$$(D_{ij} \frac{\partial\phi}{\partial x_j} + u_i \frac{\phi}{2}) = 0 \tag{3-15}$$

on the remaining portion of the boundary for $t \geq 0$.

The functional given by the Eq. 3-11 is transformed as:

$$J = \int\int_R \left\{ \frac{D_{xx}}{2} \left(\frac{\partial\phi}{\partial x}\right)^2 + D_{xy} \left(\frac{\partial\phi}{\partial x}\right)\left(\frac{\partial\phi}{\partial y}\right) + \frac{D_{yy}}{2} \left(\frac{\partial\phi}{\partial y}\right)^2 \right.$$

$$\left. + \left(\frac{u}{2} \frac{\partial\phi}{\partial x} + \frac{v}{2} \frac{\partial\phi}{\partial y}\right)\phi + \left[\frac{D_{yy}u^2 + D_{xx}v^2 - 2D_{xy}uv}{8(D_{xx}D_{yy} - D_{xy}^2)} \right]\phi^2 + \left(\frac{\partial\phi}{\partial t}\right)\phi \right\} dx\,dy \tag{3-16}$$

Eq. 3-16 also may be modified to avoid zero in the denominator of the coefficient of ϕ^2 on the right hand side. The modified form is:

$$J = \int\int_R \left\{ \frac{D_{xx}}{2} \left(\frac{\partial \phi}{\partial x}\right)^2 + D_{xy} \left(\frac{\partial\phi}{\partial x}\right)\left(\frac{\partial\phi}{\partial y}\right) + \frac{D_{yy}}{2}\left(\frac{\partial\phi}{\partial y}\right)^2 \right.$$

$$\left. + \left(\frac{u}{2}\frac{\partial\phi}{\partial x} + \frac{v}{2}\frac{\partial\phi}{\partial y}\right)\phi + \left[\frac{u^2+v^2}{8(D_L+D_d T)}\right]\phi^2 + \left(\frac{\partial\phi}{\partial t}\right)\phi \right\} dx\, dy \qquad (3\text{-}16a)$$

The proof of equivalence of the transformed functional (Eq. 3-16) and the differential Eq. 3-13 with the corresponding boundary conditions is given in Appendix B. The functional given by Eq. 3-16a is solved by the finite element method. If we let $D_{xy} = 0$ and assume the same relationships, Eq. 2-11, as used by Guymon (1970) for the dispersion coefficients, then the transformed functional represented by Eq. 3-16 reduces to the corresponding functional given by Guymon (1970).

An extension is suggested in Appendix C for solving the ground water flow equation utilizing the functional developed in this section.

3.4 Numerical approximation by the finite element method:

Consider a two-dimensional region R as shown in Fig. 3-1. For the purpose of expressing the functional in terms of a finite number of unknowns, the region R is sub-divided into a network of small triangular finite elements. In general, one should use the smallest elements in regions of maximum gradients. The dimensions of the elements in any one direction should not change abruptly. The solution for the distribution of the concentration within the region is determined by minimizing the functional, Eq. 3-16a, by the Ritz method. The generalized coordinates are selected as the concentrations at the nodal points of the triangular elements. The greater the number of the generalized coordinates (nodal points), the more accurate the result will be.

The minimization process requires the establishment of the relation for the concentration as a function of position and time. If the concentration is assumed to vary linearly with respect to the coordinates x and y over the triangular element, then we have:

$$\phi = \alpha_1 + \alpha_2 x + \alpha_3 y \tag{3-17}$$

where ϕ is defined by Eq. 3-12 and α_1, α_2 and α_3 are coefficients so determined that Eq. 3-17 reduces to the values ϕ_i, ϕ_j and ϕ_k at the nodal points i, j and k (Fig. 3-1) respectively. As an extension of and improvement over this method other higher-order polynomials should be investigated.

It is more convenient to introduce local coordinates as shown in Fig. 3-2 and defined as:

$$\xi = x - \overline{x}^m$$

$$\text{and} \quad \eta = y - \overline{y}^m$$

where $\overline{x}^m$ and $\overline{y}^m$ are the global coordinates of the centroid of the m^{th} triangular element, i.e.:

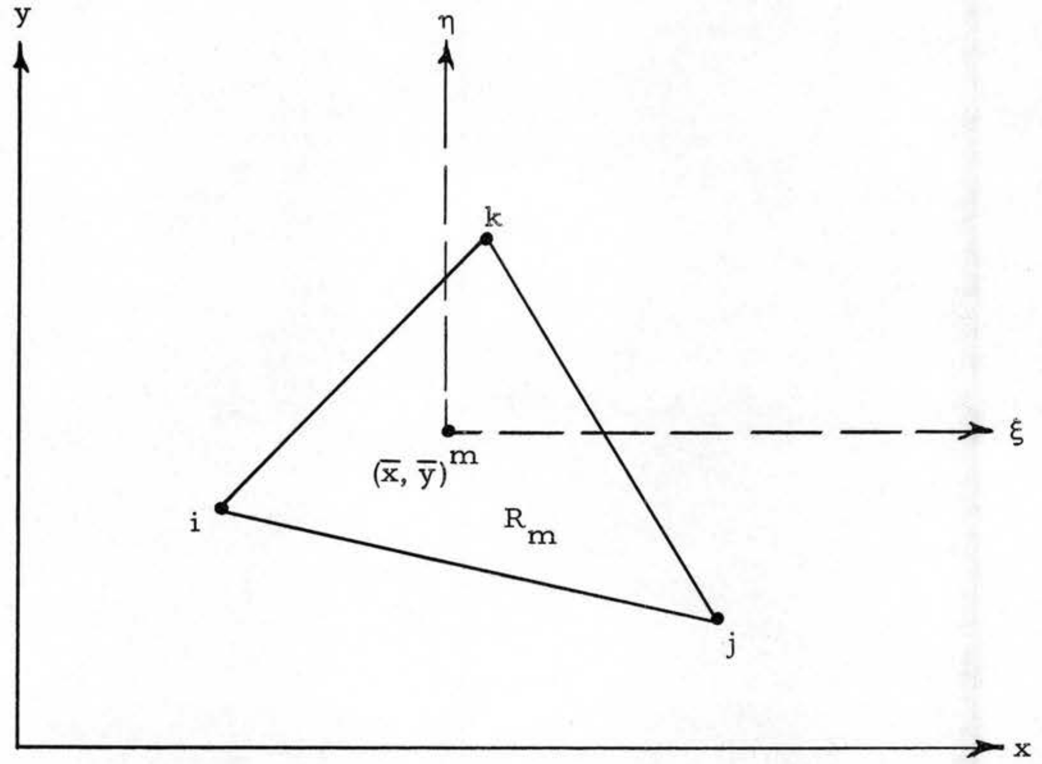


Fig. 3-2 Relation between global coordinates and local coordinates.

$$\bar{x}^m = (x_i + x_j + x_k)/3$$

and $$\bar{y}^m = (y_i + y_j + y_k)/3. \tag{3-18}$$

These local coordinates ξ and η enable us to use some of the simple integration formulas defined in Appendix D. The functional given by Eq. 3-16 is written in terms of these local coordinates as:

$$J = \int\int_R \left\{ \frac{D_{xx}}{2} \left(\frac{\partial\phi}{\partial\xi}\right)^2 + D_{xy} \left(\frac{\partial\phi}{\partial\xi}\right)\left(\frac{\partial\phi}{\partial\eta}\right) + D_{yy}\left(\frac{\partial\phi}{\partial\eta}\right)^2 \right.$$

$$+ \left(\frac{u}{2} \frac{\partial\phi}{\partial\xi} + \frac{v}{2} \frac{\partial\phi}{\partial\eta}\right) \phi$$

$$\left. + \left[\frac{D_{yy}u^2 + D_{xx}v^2 - 2D_{xy}uv}{8(D_{xx}D_{yy} - D_{xy}^2)}\right] \phi^2 + \left(\frac{\partial\phi}{\partial t}\right)\phi \right\} d\xi \; d\eta \tag{3-19}$$

and similarly Eq. 3-16a may be written as:

$$J = \int\int_R \left\{ \frac{D_{xx}}{2} \left(\frac{\partial\phi}{\partial\xi}\right)^2 + D_{xy} \left(\frac{\partial\phi}{\partial\xi}\right)\left(\frac{\partial\phi}{\partial\eta}\right) + \frac{D_{yy}}{2} \left(\frac{\partial\phi}{\partial\eta}\right)^2 \right.$$

$$\left. + \left(\frac{u}{2} \frac{\partial\phi}{\partial\xi} + \frac{v}{2} \frac{\partial\phi}{\partial\eta}\right) \phi + \left[\frac{u^2+v^2}{8(D_L + D_d T)}\right] \phi^2 + \left(\frac{\partial\phi}{\partial t}\right)\phi \right\} d\xi \; d\eta$$

(3-19a)

The concentration given by Eq. 3-17 meets continuity requirements over each finite element and the transformed value of the concentration ϕ is given by:

$$\phi = \left[A\right]\left\{\phi\right\}^m \tag{3-20}$$

where $[A]$ is a function of space only. $[A]$ is a row matrix and given in Appendix D. The three element vector $\{\phi\}^m$ is a function of time only and it represents the concentrations at each node. The superscript m denotes the m^{th} triangular element.

The nodal values of ϕ define uniquely and continuously the concentration throughout the region. The functional J given by Eq. 3-19a can now be minimized with respect to these nodal values. The minimization procedure described by Zienkiewicz and Cheung (1967) is utilized here. This process is best accomplished by evaluating, first the contributions to each differential such as $\frac{\partial J}{\partial \phi_i}$, from a typical element, then adding all such contributions and equating to zero. Only the elements adjacent to the node i will contribute to $\frac{\partial J}{\partial \phi_i}$. The contribution of the i^{th} node of the m^{th} triangular element is obtained by differentiating J given by Eq. 3-19a partially with respect to ϕ_i. The complete development is shown in Appendix D.

The final form for the differential $\frac{\partial J^m}{\partial \phi_i}$ is given as Eq. D-15 in Appendix D and repeated below:

$$\frac{\partial J^m}{\partial \phi_i} = \left(\frac{D_{xx}}{4A^m} \; a_{2i} \left[a_2\right] + \frac{D_{xy}}{4A^m} \; a_{3i} \left[a_2\right] + \frac{D_{xy}}{4A^m} \; a_{2i} \left[a_3\right] \right.$$

$$+ \frac{D_{yy}}{4A^m} \; a_{3i} \left[a_3\right] + \frac{1}{12} \; (u\, a_{2i} + v\, a_{3i}) \left[1, 1, 1\right]$$

$$+ \frac{1}{12} \; (u \left[a_2\right] + v \left[a_3\right]) + \frac{1}{16A^m} \left(\frac{u^2+v^2}{D_L+D_d T}\right)\left[(AA)_i\right] \Bigg) \; \{\phi\}^m$$

$$+ \quad \frac{\left[(AA)_i\right]}{4A^m} \left\{\frac{\partial \phi}{\partial t}\right\}^m \tag{3-21}$$

Similarly two other differentials $\frac{\partial J^m}{\partial \phi_j}$ and $\frac{\partial J^m}{\partial \phi_k}$ can also be evaluated.

Every element thus contributes to three of the differentials corresponding to the three nodes associated with it. These contributions are:

$$\left\{\frac{\partial J}{\partial \phi}\right\}^m = \begin{Bmatrix} \frac{\partial J}{\partial \phi_i} \\ \frac{\partial J}{\partial \phi_j} \\ \frac{\partial J}{\partial \phi_k} \end{Bmatrix} = \left[s\right] \{\phi\}^m + \left[p\right] \left\{\frac{\partial \phi}{\partial t}\right\}^m \tag{3-22}$$

where $\left[s\right]$ and $\left[p\right]$ are given in Appendix D as Eqs. D-23 and D-24 respectively.

The minimization procedure involves the assembly of all the differentials of J and equating these to zero. This procedure leads to the following set of simultaneous, linear, first order differential equation:

$$\left[S^*\right] \{\phi\} + \left[P^*\right] \left\{\frac{\partial \phi}{\partial t}\right\} = \{Q^*\} \qquad (3\text{-}23)$$

where $\left[S^*\right]$ is the sum of $\left[s\right]$ and $\left[P^*\right]$ is the sum of $\left[p\right]$. Both $\left[S^*\right]$ and $\left[P^*\right]$ are N by N banded, symmetric matrices, and $\{\phi\}$, $\left\{\frac{\partial \phi}{\partial t}\right\}$ and $\{Q^*\}$ are N element column matrices. The term N represents the total number of triangular nodal points over the region R . When there are no sources or sinks within the region R the $\{Q^*\}$ matrix is zero. If there are L nodal points with prescribed geometric boundary conditions, then there will be L corresponding values ϕ which are known and need not be solved.

The matrix differential equation, Eq. 3-23, is modified to eliminate the L number of equations corresponding to the geometric boundary condition nodes. Let q_n^*, $n = 1, 2, \ldots N$, be the elements of the N by one $\{Q^*\}$ matrix in Eq. 3-23. Then the $\{Q^*\}$ matrix is modified by the rule:

$$q_n = q_n^* - \sum_{\ell = 1}^{L} s_{n,\ell}\, \phi_\ell \qquad (3\text{-}24)$$

for each value of n . In Eq. 3-24, $s_{n,\ell}$ are the elements of the $\left[S^*\right]$ matrix and q_n represents the elements of the modified, N by one $\{Q^*\}$ column matrix $\{Q^*\}$. Then the rows and columns of the matrices $\left[S^*\right]$ and $\left[P^*\right]$ of Eq. 3-23 are set equal to zero on the ϕ_L points and also the L rows of $\{Q^*\}$ matrix are set equal to zero. Finally the matrices $\left[S^*\right]$, $\left[P^*\right]$ and $\{Q^*\}$ of Eq. 3-23 are modified by shifting the lower non-zero values up or to the left until the L number of columns and rows have been eliminated.

Denoting the modified matrices as $\left[S\right]$, $\left[P\right]$ and $\{Q\}$ corresponding to the matrices $\left[S^*\right]$, $\left[P^*\right]$, and $\{Q^*\}$ respectively in Eq. 3-23, the following equation is obtained:

$$\left[S\right]\{\phi\} + \left[P\right]\left\{\frac{\partial\phi}{\partial t}\right\} = \{Q\} \qquad (3\text{-}25)$$

where $\left[S\right]$ and $\left[P\right]$ are (N-L) by (N-L) banded, symmetric matrices and $\{\phi\}$, $\left\{\frac{\partial\phi}{\partial t}\right\}$ and $\{Q\}$ are (N-L) element column matrices. The variational principle incorporates the natural boundary conditions corresponding to Eq. 3-5 in the functional. A proof is given in Appendix E to show that the system of equations represented by Eq. 3-22 is independent of the coordinates.

In this chapter, the mathematical model describing the transient concentration distribution in a two-dimensional case is presented, Eqs. 3-3, 3-4 and 3-5. Utilizing the variational principles and the finite element method, a numerical simulator of the mathematical model is developed, Eq. 3-25. The numerical solutions of the simulator are given in Chapter IV.

CHAPTER IV

APPLICATION OF THE NUMERICAL SIMULATOR AND DISCUSSION OF THE RESULTS

The primary objectives of this research were to evaluate the significance of the mixed partial derivatives in the new functional, Eq. 3-11, and the use of Eq. 3-2 which treats the hydrodynamic dispersion as an anisotropic quantity. Solution of the resulting set of simultaneous, linear, first order differential equations represented by Eq. 3-25 was obtained in the same manner as described by Guymon (1970). The following paragraphs describe the procedure for using the numerical simulator and give an evaluation of the results obtained.

4.1 Bandwidth of the matrices of the simulator:

The symmetric and banded characters of the matrices $[S]$ and $[P]$ of Eq. 3-25 are taken advantage of in storing the elements. Only the upper triangular bands of the matrices are stored to conserve computer storage. The maximum non-zero elements in any row of the matrices $[S]$ and $[P]$ will be equal to the adjacent nodes with which the node corresponding to the row of the matrices is connected plus one. This indicates that a certain numbering of the nodes will give the minimum bandwidth. Here, the term "bandwidth" for any row is defined to include the main diagonal and the elements to the right of the main diagonal including the last non-zero element. This rule is applied to each row of the matrices and the maximum value obtained from any one row of the matrices is taken as the bandwidth for the whole system, Eq. 3-25. Guymon (1970) gives a brief description for the most effective numbering scheme to obtain a minimum bandwidth.

4.2 Method of solution of the system of linear differential equations:

The simultaneous, linear, first order differential equations represented by Eq. 3-25 can be written as:

$$\left[P\right] \left\{\frac{\partial \phi}{\partial t}\right\} = - \left[S\right] \{\phi\} + \{Q\} \tag{4-1}$$

Using the initial values of ϕ_i, $i = 1, 2, \ldots (N-L)$, the right hand side of Eq. 4-1 can be combined to yield:

$$\left[P\right] \left\{\frac{\partial \phi}{\partial t}\right\} = \{F\} \tag{4-2}$$

Eq. 4-2 is solved for the vector $\dot{\underset{\sim}{\phi}} = \left\{\frac{\partial \phi}{\partial t}\right\}$ using the well known "Gaussian elimination" method. The resulting set of first order differential equations are numerically integrated using a fourth order Runge-Kutta technique to develop the necessary starting values followed by the application of the Adams-Moulton multistep predictor-corrector method. Algorithms for these methods are given in Conte (1965) and the formulas used in this simulator are given in Appendix F.

The values computed by using the Adams-Moulton multistep predictor-corrector formulas, Eqs. F-4 and F-5 given in Appendix F, are used to find the local truncation error $\{\epsilon\}_{n+1}$ which is calculated as:

$$\{\epsilon\}_{n+1} = -\frac{1}{14}\left(\{\phi\}^{(1)}_{n+1} - \{\phi\}^{(0)}_{n+1}\right) \tag{4-3}$$

Depending upon the accuracy required and the type of problem, values are read in as input data specifying the maximum and minimum permissible error. If the absolute value of ϵ_{n+1} is greater than the specified maximum error, provision is made in the computer program to automatically reduce the time step size by half. If the maximum absolute value of ϵ_{n+1} is less than the specified minimum error, the time step size is doubled. This adjustment in time step size is made to reduce computer time.

Solutions for the concentration distribution are repeated for each time increment until the whole time interval is completed. At any instant in time, the concentration C may be obtained by taking an inverse transformation of ϕ using Eq. 3-12.

The computer program: The computer program was written in Fortran IV language. The program developed in this study has been adopted from a modification of a previous program reported by Guymon (1970). It consists of five segments and a number of subroutines for solving the system of linear, first order differential equations. Labeled common blocks are used to conserve storage and to minimize time. A brief description of each of the five segments is given in Appencix G. A flow chart, method of data preparation and a listing of the program are also given in Appendix G.

4.3 Results and discussion:

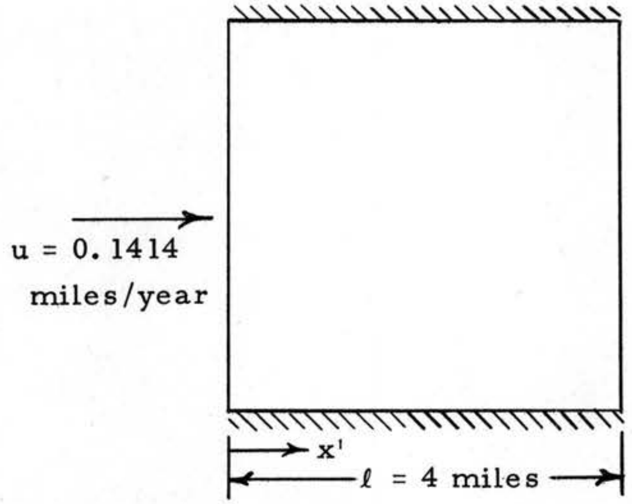
Types of problems solved and means for comparison: The numerical simulator developed in Chapter III, Eq. 3-25, is capable of solving a general two-dimensional dispersion equation having mixed partial derivatives. The simulator was also used to solve a one-dimensional case, say in the x-direction, assuming the component of the velocity v and the partial derivatives in the y-direction equal zero. The one-dimensional equation is similar to Eq. 2-6. The advantage of transforming the two-dimensional equation into a one-dimensional form is that we have analytic solutions for the one-dimensional case, Eq. 2-7, to compare with the numerical results.

The one-dimensional problems were also transformed into two-dimensional forms by a suitable rotation of axes and coordinates. In this way the numerical simulator, Eq. 3-25, which is applicable to a two-dimensional case was used without any modification and the results compared with the analytical solutions given by Eq. 2-7. The results were also compared with other finite element solutions using different functionals.

Comparison of results from previous related work: Guymon (1970) used the variational principles and the finite element method to solve the dispersion equation excluding the mixed partial derivatives and solved steady flow problems. The problem shown in Fig. 4-1 is identical to that solved by Guymon (1970). The region was divided into 16 triangular elements as shown in Fig. 4-2. The analytic results are presented at selected values of the fractional distance x'/ℓ in column 2 of Table I.

Results from different computers: Before proceeding with the use of the new functional, Eq. 3-11, to solve the problem, it was necessary to evaluate the difference in the results obtained by solving the same problem with two different computers. Guymon (1970) solved the two-dimensional case for the boundary conditions shown in Fig. 4-1 and for the element configurations shown in Fig. 4-2, using an IBM 7044 computer. His results are given in column 3 of Table I. Using Guymon's functional, the same problem was solved using a CDC 6400 computer and the results are given in column 4 of Table I. The discrepancy in the two results may be attributed to the fact that IBM 7044 and CDC 6400, respectively, carry 16 and 29 significant digits in double precision resulting in different roundoff errors.

Rotation of axes: An attempt was made as shown in Chapter III to eliminate the mixed partial derivatives from Eq. 3-3 by rotating the coordinates so that the functional developed by Guymon (1970) could be utilized. The resulting equation (Eq. 3-6) is in terms of $x'y'$ coordinates. The problem in Figs. 4-1 and 4-2 was reformulated utilizing the new coordinates x' and y' as shown in Fig. 4-2. The



I.C.: $C/C_o = 0$ at $t = 0$ for $0 < x' < \ell$

B.C.: $C/C_o = 1$ at $t \geq 0$ for $x' = 0$

$C/C_o = 0.148$ at $t \geq 0$ for $x' = \ell$

$D_L = 470\ cm^2/sec$

Fig. 4-1 One-dimensional column of porous media.

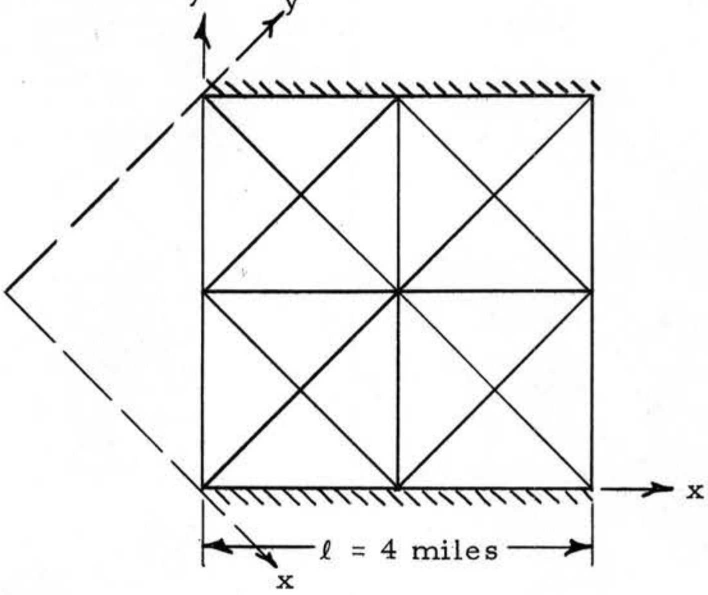


Fig. 4-2 Two-dimensional grid network with 16 elements for problem shown in Fig. 4-1.

TABLE I

VALUES OF C/C_o FOR PROBLEM IN FIGURES 4-1 AND 4-2 AT TIME = 5 YEARS

LONGITUDINAL DISPERSION COEFFICIENT D_L = 470 CM^2/SEC

Fractional Distance x'/ℓ	Analytical Solutions (Eq. 2-7)	Results Using the Functional Developed by Guymon (1970)			Results Using New Functional Including Mixed Partial Derivatives		
		Guymon's Method		Mixed Partials Eliminated by Rotation of Axes	Ratios of Lateral to Longitudinal Dispersion Coefficients		
		IBM 7044	CDC 6400		$D_T/D_L=0.0$	$D_T/D_L=0.05$	$D_T/D_L=0.1$
1	2	3	4	5	6	7	8
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.25	0.755	0.787	0.788	0.750	0.750	0.754	0.757
0.5	0.503	0.526	0.527	0.522	0.522	0.522	0.522
0.75	0.294	0.340	0.341	0.298	0.298	0.302	0.306
1.0	0.148	0.148	0.148	0.148	0.148	0.148	0.148

numerical results are given in column 5 of Table I. The coordinate transformation includes the effect of the mixed partial derivatives and a comparison of columns 4 and 5 of Table I indicates the contribution due to the mixed partial terms. For this problem, the results obtained from Eq. 3-6 which includes the effect of the mixed partial derivatives appear to be closer to the analytic solutions than that obtained by using Guymon's (1970) functional. For the type of relationships considered with the dispersion coefficients (Eq. 3-2), this rotation technique can be used for uniform velocity distributions, but cannot be used for non-uniform flow patterns. Both steady and unsteady cases can be handled.

Results using new functional: The new functional, Eq. 3-11, which includes the mixed partial derivatives, was used to solve the same problem (Figs. 4-1 and 4-2). Shamir and Harleman (1967) report that the lateral dispersion coefficient D_T is in the range of (0.05 to 0.1) times the longitudinal dispersion coefficient D_L . Utilizing the new functional, numerical results were computed for ratios of $D_T/D_L = 0.0$, 0.05, and 0.1 as presented in columns 6, 7 and 8 respectively of Table I. Considering the coarse element sizes and the type of linear approximations used for the concentration, the numerical results compare favorably with the analytical solutions, and better than the results obtained by Guymon (1970) using the functional without the mixed partial derivatives. From the results given in Table I, it appears that the lateral dispersion coefficient D_T has very little effect upon the concentration distribution.

The values of the concentration as a function of time for different values of the fractional distance are plotted in Fig. 4-3. Three sets of results are plotted on the same figure. In one set, the concentrations were computed after elimination of the mixed partial terms by rotation of axes. The lateral dispersion and diffusion were neglected in this case. In the next two sets ratios of $D_T/D_L = 0.0$ and 0.05 were used and molecular diffusion was neglected. In all three cases, the dispersion coefficients were computed using the relationships given by Eq. 3-2. The three sets of results are very nearly equal.

The following points may be noted. Though there is provision to include the molecular diffusion D_d in Eq. 3-2, it was assumed to be negligible in all the problems discussed in this study. The effect of molecular diffusion is further discussed in section 4.4.

The longitudinal dispersion coefficient, D_L, used in Eq. 2-7 by Guymon was about 470 cm^2/sec. This value is extremely large for most porous media (Shamir and Harleman, 1967), but was probably needed to eliminate stability problems in the numerical technique used for the solution of Eq. 3-25. This stability problem is discussed later in section 4.4.

The problem shown in Fig. 4-1 was again solved by dividing the region into smaller triangles as shown in Fig. 4-4. The solutions

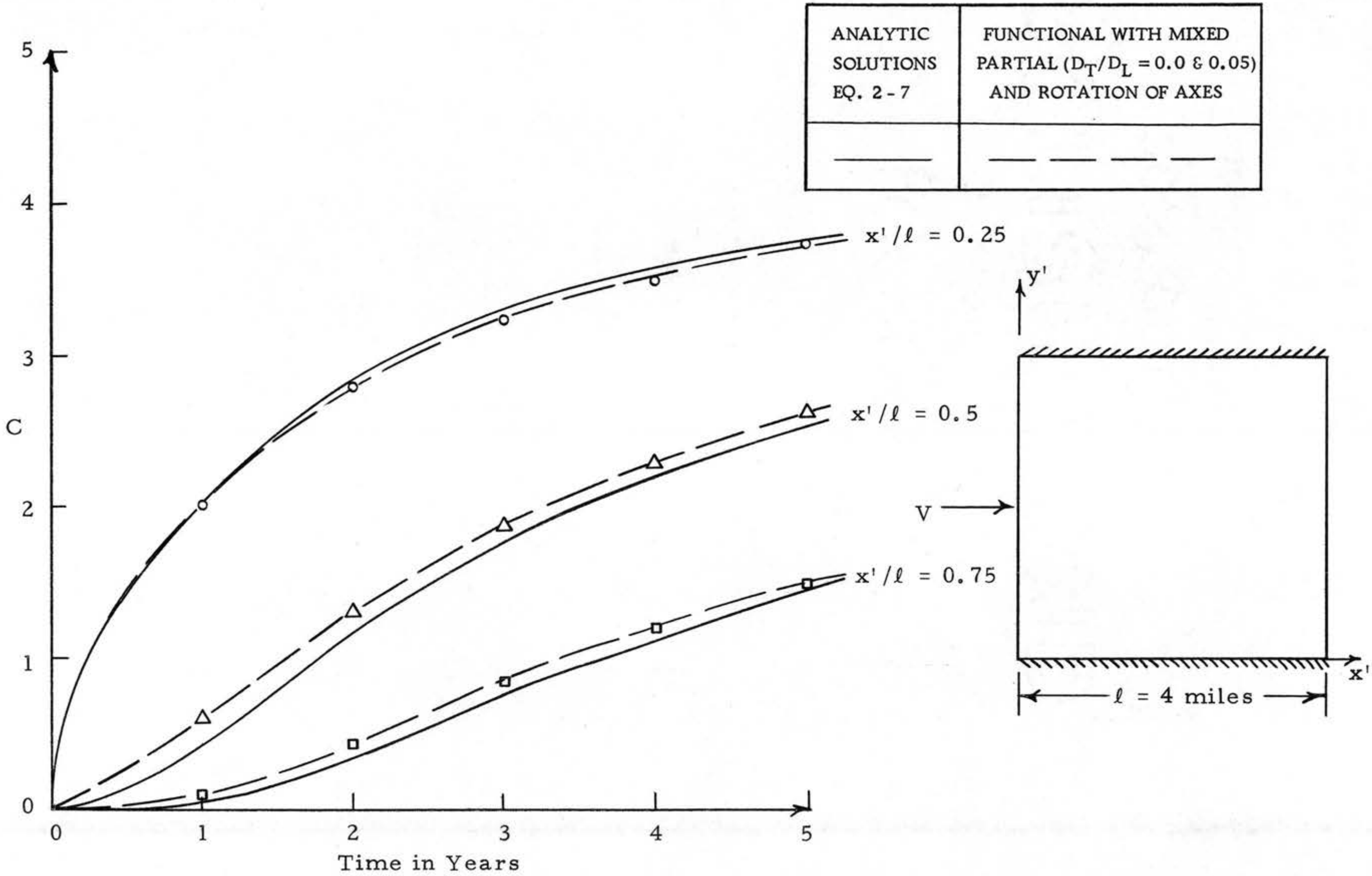


Fig. 4-3 Analytical and numerical results for problem in Fig. 4-2.

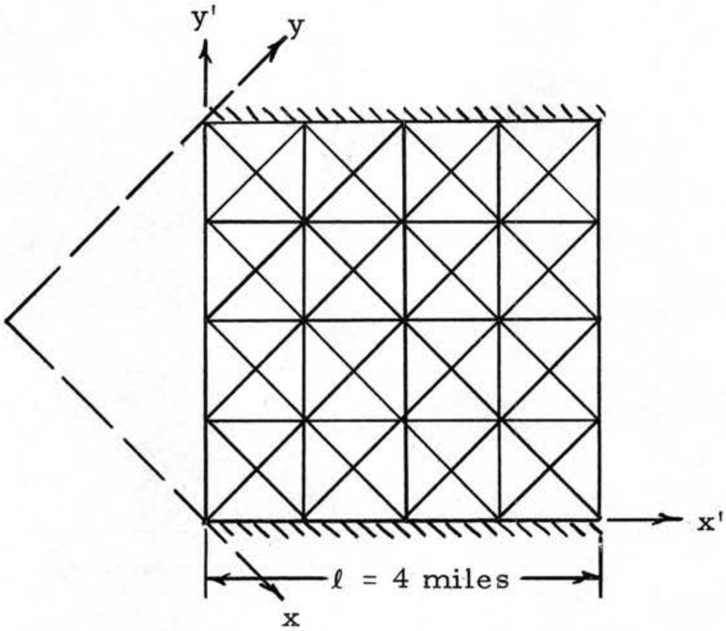


Fig. 4-4 Two-dimensional grid network with 64 elements for problem shown in Fig. 4-1.

were obtained in the same manner as described for solving the problem in Fig. 4-2. The analytic results are given in column 2 of Table II and the numerical results obtained by Guymon (1970) are given in column 3. Results were also obtained using Guymon's method and rotated coordinates to account for the mixed partial derivatives as given in column 4 of Table II. Numerical results were computed using the new functional with mixed partial derivatives for ratios of $D_T/D_L = 0.0$ and 0.05 and are presented in columns 5 and 6 respectively of Table II. For some values of the fractional distance x'/ℓ , the numerical results obtained by using the functional with mixed partial derivatives are closer to the analytical results than that reported by Guymon (1970), and for other points not so close. When stability requirements are satisfied, it appears from this problem that decreasing the area of the elements does not improve the results significantly. For stable problems the decrease in the area of the elements caused by an increase in the number of the nodal points might introduce greater round-off errors in solving larger matrices.

Observations: The numerical results obtained for the problems shown in Figs. 4-1, 4-2 and 4-4 indicate that Eq. 3-3 truly represents the two-dimensional mathematical model for describing the transient concentration distribution. The lateral dispersion is properly accounted for by Eq. 3-3. The stability of the system represented by Eq. 3-25 is an important aspect in obtaining correct solutions. This stability aspect is discussed in section 4.4.

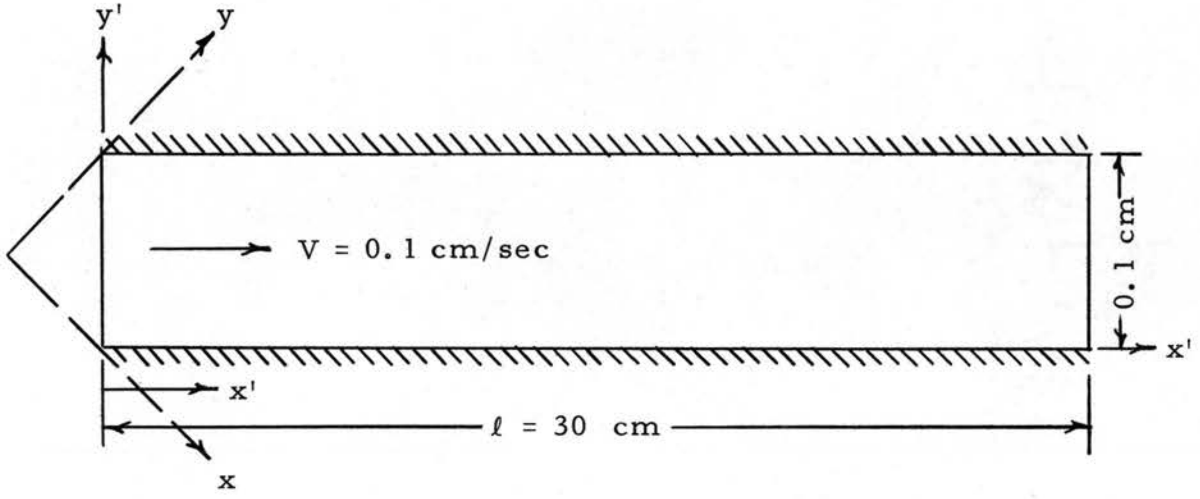
TABLE II

VALUES OF C FOR PROBLEM IN FIGURES 4-1 AND 4-4 AT TIME = 5 YEARS

Fractional Distance x'/ℓ	Analytical Solutions (Eq. 2-7)	Results Using the Functional Developed by Guymon (1970)		Results Using New Functional Including Mixed Partial Derivatives	
		Guymon's Method	Mixed Partials Eliminated by Rotation of Axes	Ratios of Lateral to Longitudinal Dispersion Coefficients	
				$D_T/D_L=0.0$	$D_T/D_L=0.05$
1	2	3	4	5	6
0	5.0	5.0	5.0	5.0	5.0
0.125	4.405	4.407	4.373	4.373	4.376
0.25	3.775	3.723	3.720	3.721	3.721
0.375	3.085	3.080	3.017	3.018	3.024
0.5	2.515	2.415	2.421	2.422	2.423
0.625	1.955	1.909	1.845	1.846	1.853
0.75	1.470	1.430	1.435	1.436	1.436
0.875	1.065	1.087	1.057	1.057	1.061
1.0	0.741	0.741	0.741	0.741	0.741

Application of the simulator to column problems: Concentration distributions in a long column shown in Fig. 4-5 were evaluated using the analytic solution (Eq. 2-7) and the finite element technique. Table III and Figs. 4-6 and 4-7 include the results for a column 30 cm long having a steady state seepage velocity of 0.1 cm/sec. Analytic solutions for concentration at both 10 and 20 seconds after introducing the tracer are given in columns 2 and 5 respectively of Table III.

The finite element model for the two-dimensional case was used in two different ways in the solution of this problem. Initially, the coordinate axes were chosen so that the x'-axis corresponded to the longitudinal axis of the column and the velocity component and the dispersion coefficients in the y'-direction were assumed as zero. This would represent a one-dimensional problem and the results are given in columns 3 and 6 of Table III. To test the two-dimensional capabilities of the technique, the coordinate axes were rotated 45° and the solutions recalculated as tabulated in columns 4 and 7 of Table III. In this latter case, $u = v = V/\sqrt{2}$ where V is the seepage velocity in the column and u and v are the components of seepage velocity respectively in the x and y directions. Note that the results in Table III, columns 3 and 4 and also 6 and 7, rounded to two significant digits are identical for the one and two-dimensional solutions. The numerical and analytic solutions are quite similar, as shown graphically in Figs. 4-6 and 4-7, thus verifying the validity



I.C.: $C/C_o = 0$ at $t = 0$ for $0 \leq x' \leq \ell$

B.C.: $C/C_o = 1.0$ at $t \geq 0$ for $x' = 0$

$$\frac{\partial C}{\partial x'} = 0 \quad \text{at } t \geq 0 \quad \text{for } x' = \ell$$

$$D_L = 1.0 \ \text{cm}^2/\text{sec}$$

Fig. 4-5 Long narrow column of porous media.

TABLE III

VALUES OF C/C_o FOR PROBLEM IN FIGURE 4-5

ℓ = 30.0 cm; width = 0.1 cm   V = 0.1 cm/sec D_L = 1.0 cm^2/sec

Fractional Distance	C/C_o at t = 10 secs			C/C_o at t = 20 secs		
x'/ℓ	Analytical (Eq. 2-7)	Numerical One-Dim.	Numerical Two-Dim.	Analytical (Eq. 2-7)	Numerical One-Dim.	Numerical Two-Dim.
1	2	3	4	5	6	7
0	1.00	1.00	1.00	1.00	1.00	1.00
0.1	0.58	0.61	0.61	0.73	0.74	0.74
0.2	0.24	0.31	0.31	0.45	0.49	0.49
0.3	0.07	0.07	0.07	0.24	0.25	0.25
0.4	0.01	0.02	0.02	0.10	0.12	0.12
0.5	0	-0.01	-0.01	0.04	0.03	0.03
0.6	0	0	0	0.01	0.01	0.01
0.7	0	0	0	0	0	0
.	.	.	.	.	.	.
.	.	.	.	.	.	.
1.0	0	0	0	0	0	0

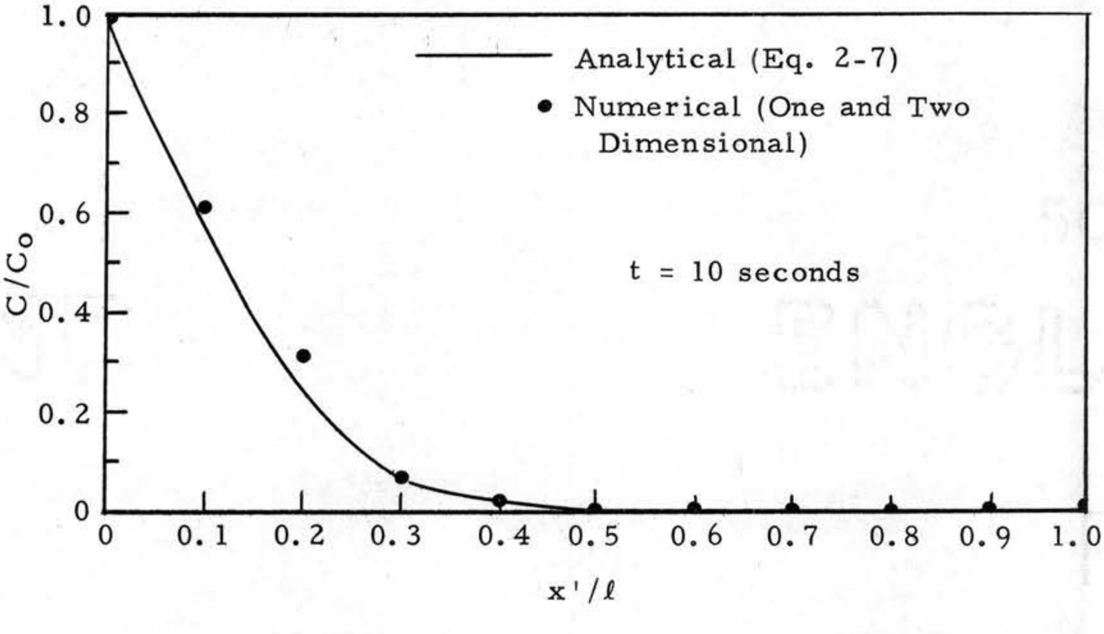


Fig. 4-6 Analytic and numeric solutions for problem in Fig. 4-5.

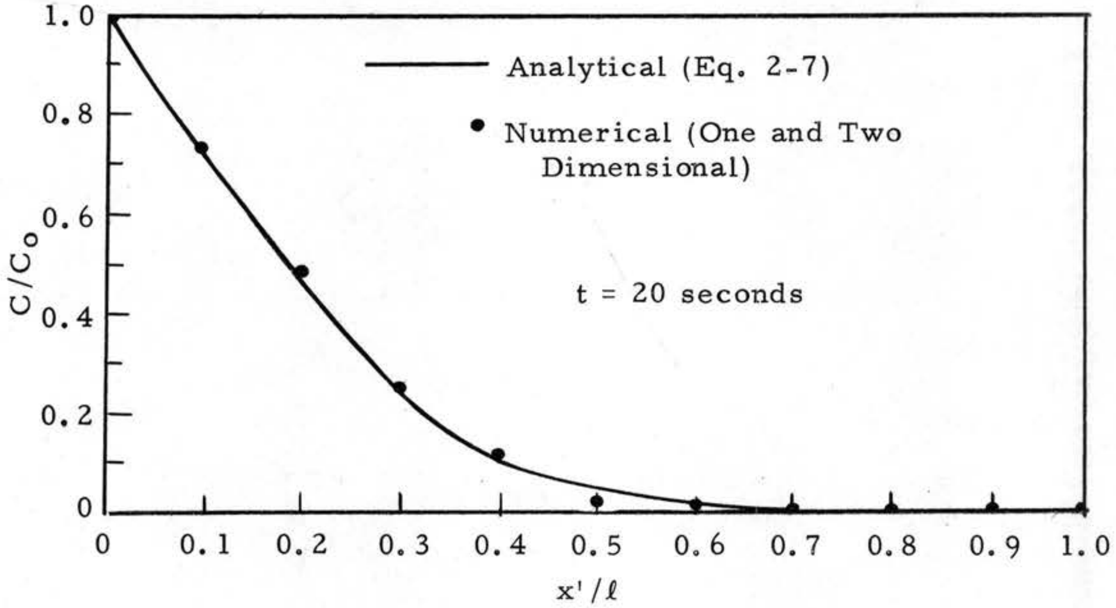
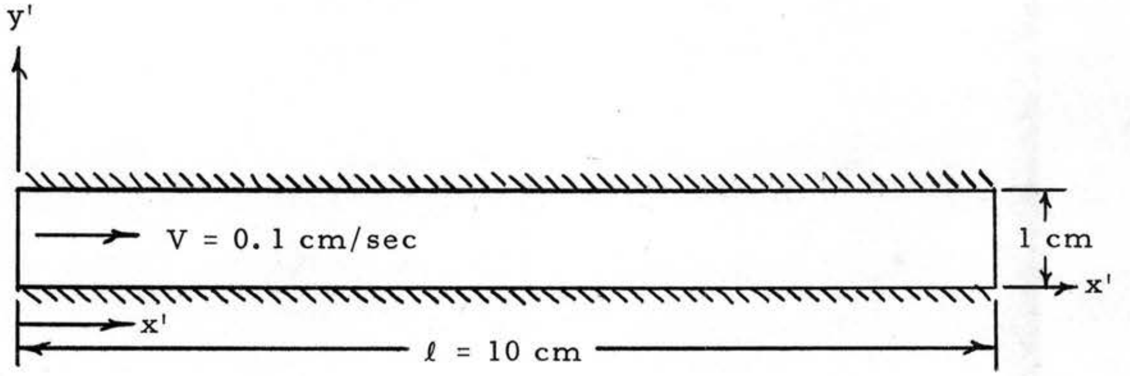


Fig. 4-7 Analytic and numeric solutions for problem in Fig. 4-5.

of the finite element technique. For both the 10 and 20-second solutions, the contaminates have not moved more than two-thirds of the column length and the exit boundary condition $\frac{\partial C}{\partial x'} = 0$ is satisfied.

It should be noted in Table III that at $x'/\ell = 0.5$ and $t = 10$ secs, the value of the concentration is negative. This is a result of instability in the approximate solution of Eq. 3-16a. The instability is due to the illconditioned nature of the $[S]$ matrix of Eq. 3-25. For the type of problems solved, the solutions appear to be stable when all the elements of the (N-L) by one column matrix $\{F\}$ on the right hand side of Eq. 4-2 are positive at the starting time. This depends upon the off-diagonal elements of the $[S^*]$ matrix of Eq. 3-23. Parameters influencing the element values of this $[S^*]$ matrix include the seepage velocity, grid network layout, and most significantly the longitudinal dispersion coefficient D_L.

The stability problem is further demonstrated by Figs. 4-9, 4-10 and 4-11 which are solutions to the problem depicted in Fig. 4-8. The problem, assumed to be one-dimensional, was solved using the following values for D_L: 0.01, 0.20, 0.40, and 6.0 cm^2/sec. For $D_L = 0.01$ cm^2/sec, the solution was unstable because the $[S]$ matrix of Eq. 3-25 becomes ill-conditioned and instability is introduced in the numerical solution. The results are given in Appendix H to show the magnitude of the unstable conditions. Instability also occurred for both $D_L = 0.20$ and 0.40 cm^2/sec as shown by Figs. 4-9 and 4-10



I.C.: $C/C_o = 0$ at $t = 0$ for $0 < x' \leq \ell$

B.C.: $C/C_o = 1.0$ at $t \geq 0$ for $x' = 0$

$$\frac{\partial C}{\partial x'} = 0 \quad \text{at } t \geq 0 \quad \text{for } x' = \ell$$

$D_L = 0.01, 0.2, 0.4$ and $6.0\ cm^2/sec$

Fig. 4-8 One-dimensional column of porous media.

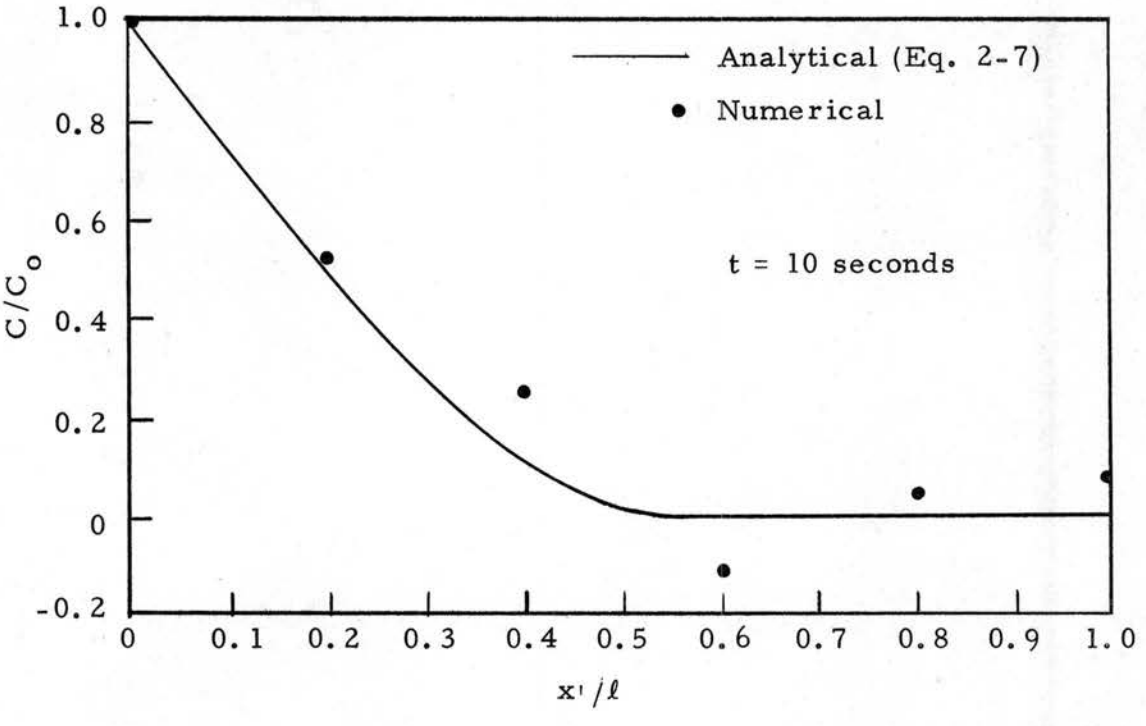


Fig. 4-9 Analytic and numeric solutions for problem in Fig. 4-8 for $D_L = 0.2\ cm^2/sec$.

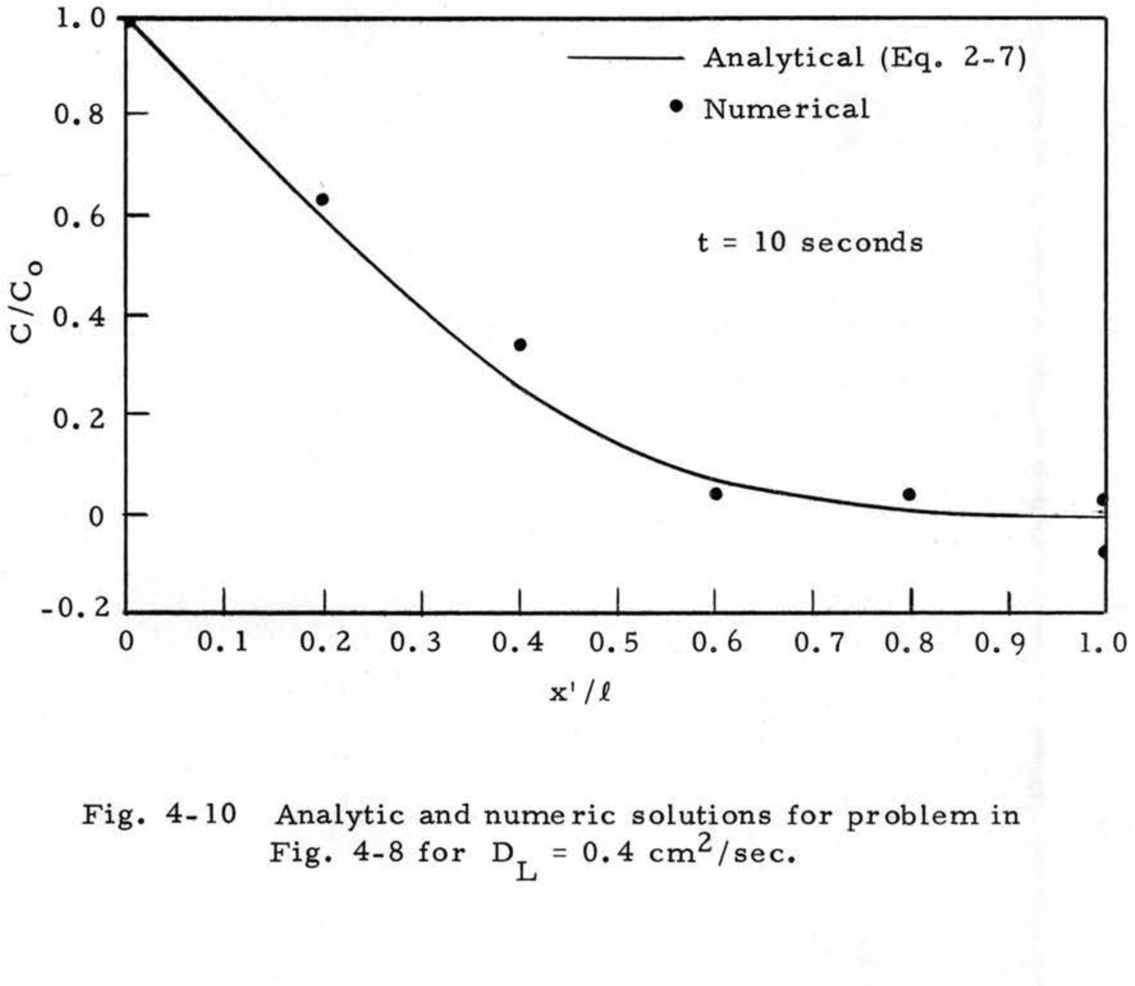


Fig. 4-10 Analytic and numeric solutions for problem in Fig. 4-8 for $D_L = 0.4\ cm^2/sec$.

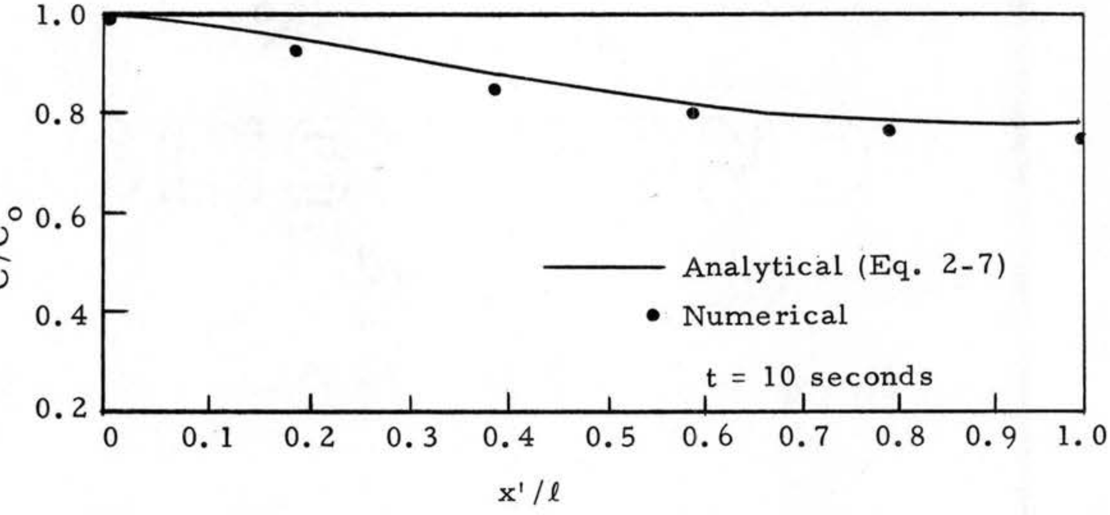
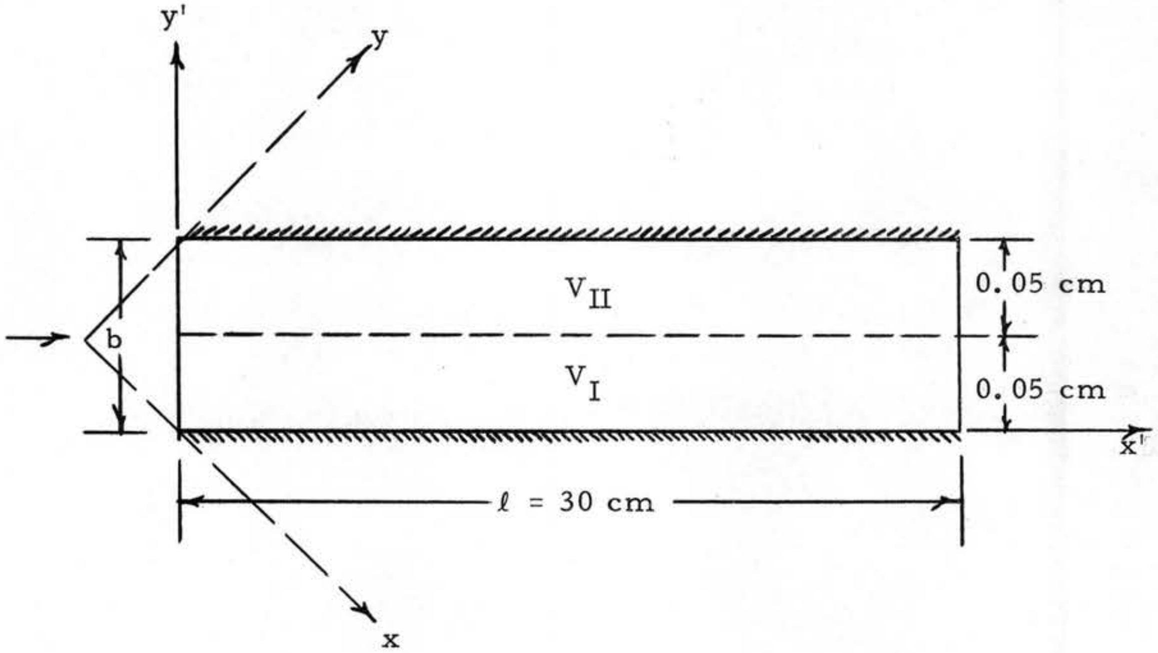


Fig. 4-11 Analytic and numeric solutions for problem in Fig. 4-8 for $D_L = 6.0\ cm^2/sec$.

where the numerical values oscillate on both sides of the analytic solutions. Note the oscillations are much less pronounced for $D_L = 0.40\ cm^2/sec$. This, in conjunction with the results shown in Figs. 4-6 and 4-7 suggests that the numerical solutions converge on the analytic solutions as the value of D_L increased. For $D_L = 6.0\ cm^2/sec$, as shown in Fig. 4-11, the results were stable. The stability criteria is discussed further later.

The inflow boundaries for the problems in Figs. 4-5 and 4-8 were fixed at a given concentration level. All other boundaries were treated as natural boundary conditions $\frac{\partial C}{\partial n} = 0$ and this is referred to as a reflection condition by Shamir and Harleman (1967). The numerical solutions shown in Fig. 4-11 corresponds to a value of the longitudinal dispersion coefficient $D_L = 6.0\ cm^2/sec$ and the contaminate has moved the full length of the column in the 10 seconds time. In this case, the exit boundary condition $\frac{\partial C}{\partial n} = 0$ is not satisfied. Since the functional requires that there be no concentration gradient across the exit boundary, $\frac{\partial C}{\partial n} = 0$, it is necessary to use the principles of the method of images to develop the necessary concentration gradients which can be superimposed resulting in a zero gradient across the exit boundary. The analytic solution shown in Fig. 4-11 is the resultant after superimposing the results obtained using Eq. 2-7 for a finite length of the porous medium.

Unsteady and non-uniform flow cases: The generality of the new functional provides for solution of problems in unsteady and



I.C.: $C/C_o = 0$ at $t = 0$ for $0 \leq x' \leq \ell$

B.C.: $C/C_o = 1.0$ at $t \geq 0$ for $x' = 0$

$$\frac{\partial C}{\partial x'} = 0 \text{ at } t \geq 0 \text{ for } x' = \ell$$

$D_L = 1.0\ cm^2/sec$

Fig. 4-12 Long narrow column of porous media with different velocities V_I and V_{II}.

of the seepage velocities in the two parts are different. One way to have different seepage velocities V_I and V_{II} in parts I and II respectively is to have different values for the porosity of the materials. The reason to have just two different seepage velocities is that we can compare the numerical results and the analytic solutions corresponding to a single uniform velocity for the whole region equal to the average of V_I and V_{II}.

Numerical results were obtained for two cases. In case (1), the seepage velocity V_I in part I was assumed as 0.08 cm/sec and V_{II} in part II as 0.12 cm/sec, thus maintaining an average velocity of 0.1 cm/sec for the whole region. The corresponding velocity components u and v in the directions x and y respectively were calculated and used in the computation of the dispersion coefficients and also used as flow parameters. The numerical results were computed at time levels equal to 10 seconds and 20 seconds and given in Table IV for various values of y'/b at different points along the length ℓ. For both the 10 and 20-second solutions, the exit boundary condition $\frac{\partial C}{\partial n} = 0$. As in the uniform flow case, here also for $t = 10$ second solution at $x'/\ell = 0.5$ due to instability, the value of the concentration is negative.

In case (2), the seepage velocity V_I in part I was assumed as 0.05 cm/sec and V_{II} in part II as 0.15 cm/sec thereby maintaining an average velocity of 0.1 cm/sec for the whole region. The

TABLE IV

VALUES OF C/C_o FOR PROBLEM IN FIG. 4-12

Case (1) $V_I = 0.08$ cm/sec; $V_{II} = 0.12$ cm/sec

$\ell = 30.0$ cm; $b = 0.1$ cm; $D_L = 1.0\ cm^2/sec$

Fractional Distance x'/ℓ	C/C_o at t = 10 secs. y'/b					C/C_o at t = 20 secs. y'/b				
	0	0.25	0.5	0.75	1.0	0	0.25	0.5	0.75	1.0
0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
0.1		0.59		0.62			0.72		0.76	
0.2	0.29		0.31		0.32	0.47		0.49		0.51
0.3		0.07		0.08			0.23		0.27	
0.4	0.02		0.02		0.02	0.11		0.12		0.13
0.5		0		-0.01			0.03		0.04	
0.6	0		0		0	0.01		0.01		0.01
0.7		0		0			0		0	
0.8	0		0		0	0		0		0
0.9		0		0			0		0	
1.0	0		0		0	0		0		0

computations were similar to those in case (1) described in the previous paragraph. The results are given in Table V.

It is to be noted that in both cases, the average value of the concentration at any value of the fractional distance x'/ℓ is approximately equal to the concentration obtained at the corresponding points in Fig. 4-5 and given in Table III under uniform flow conditions. This is given as a partial proof of the validity of the results obtained using different velocity distributions.

In a strictly steady, non-uniform flow the seepage velocity is the only quantity which varies between different elements, for all other conditions remaining the same. Corresponding to the seepage velocity in each finite element, the x and y components can be computed and read in as data for the numerical simulator. In this way, the simulator could be used to solve for the concentrations when the velocity distribution is either uniform or non-uniform.

It should be noted that for unsteady flow, the dispersion coefficients will change with respect to time. This will involve the computation of a new $\left[S\right]$ matrix in Eq. 3-25 for each time step requiring additional computer time.

4.4 Stability criteria and convergence of the solution:

The finite element method has been very widely used and shown to be stable and convergent for structural analysis and steady state problems. In the present study, a stable solution for the time

TABLE V

VALUES OF C/C_o FOR PROBLEM IN FIG. 4-12

Case (2) $V_I = 0.05$ cm/sec; $V_{II} = 0.15$ cm/sec
$\ell = 30$ cm; $b = 0.1$ cm; $D_L = 1.0\ cm^2/sec$

Fractional Distance x'/ℓ	C/C_o at t = 10 secs. y'/b					C/C_o at t = 20 secs. y'/b				
	0	0.25	0.5	0.75	1.0	0	0.25	0.5	0.75	1.0
0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
0.1		0.57		0.65			0.69		0.78	
0.2	0.27		0.31		0.35	0.44		0.49		0.55
0.3		0.06		0.09			0.20		0.30	
0.4	0.01		0.02		0.02	0.10		0.12		0.15
0.5		0		-0.01			0.02		0.04	
0.6	0		0		0	0.01		0.01		0.01
0.7		0		0			0		0	
0.8	0		0		0	0		0		0
0.9		0		0			0		0	
1.0	0		0		0	0		0		0

dependent concentration distribution is sought by the following approach. At first we discretize only the space variables by the finite element method leaving the time variable continuous. The resulting system of ordinary differential equations can be numerically integrated with respect to the time variable to obtain the solutions at the end of discrete time steps. Then the stability criteria of the system of equations are studied in the semi-discrete form.

Stability of the system: The system of equations to be solved is represented by Eq. 3-25 which can be written as Eq. 4-1 and repeated below:

$$[P] \left\{ \frac{\partial \phi}{\partial t} \right\} = - [S] \{\phi\} + \{Q\} \tag{4-1}$$

where $\phi = \phi(t)$ at any point in space.

Eq. 4-1 is comparable to the Eq. 8-8 (page 253) of Varga (1962), if we assume that the source term $S(x, y; t)$ of the system of equations given by Varga is time-independent and the vector $\overline{\tau}(t)$ is negligible. In Eq. 4-1, the matrices $[P]$ and $[S]$ are time-independent entries and the initial values of the concentrations are equal to $\phi(0)$. For the general case of a system of differential equations represented by Eq. 4-1, the matrices $[P]$ and $[S]$ should satisfy certain conditions which are discussed below.

The maximum number of non-zero entries in any row i of the $[P]$ and $[S]$ matrices of Eq. 4-1 are equal to the number of adjacent nodal points with which the node corresponding to the row i is connected plus one. The $[P]$ matrix should be non-singular and diagonally dominant with positive diagonal entries.

According to Varga (1962), the (N-L) by (N-L), real, symmetric $[S]$ matrix of Eq. 4-1 should be irreducibly diagonally dominant with non-positive off-diagonal entries. The concept of irreducibility may be interpreted geometrically (Varga, 1962, Section 1.4). Let $[S] = (a_{i,j})$ be any square matrix of size $n \times n$ and consider any n distinct points $P_1, P_2, \ldots, P_n$ in the plane and denote these n points as nodes. For every non-zero entry $a_{i,j}$ of the $[S]$ matrix, the node P_i may be connected to the node P_j by means of a path $\overrightarrow{P_iP_j}$, directed from P_i to P_j as shown in Fig. 4-13. In this way, with every $n \times n$ matrix $[S]$ can be associated a finite directed graph. A directed graph is strongly connected if, for any ordered pair of nodes P_i and P_j there exists a directed path:

$$\overrightarrow{P_iP_{\ell_1}}, \ \overrightarrow{P_{\ell_1}P_{\ell_2}}, \ \ldots, \ \overrightarrow{P_{\ell_{r-1}}P_{\ell_r=j}}$$

Fig. 4-13. Directed graph from P_i to P_j.

connecting P_i to P_j where each of the points $\ell_1, \ell_2, \ldots, \ell_{r-1}$ may be any one excluding i and j among the n points. The matrix is irreducible if it has a strongly connected directed graph. For reducible matrices the associated directed graph is not strongly connected. Another property is that all the off-diagonal entries of any row or column of a matrix cannot vanish if the matrix is irreducible (Varga, 1962).

Varga defines the n x n matrix $[S] = (a_{i,j})$ as irreducibly diagonally dominant if it is:

i. irreducible as defined above;

and ii. $$|a_{i,i}| \geq \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{i,j}| \qquad (4\text{-}4)$$

for all $1 \leq i \leq n$, with strict inequality in Eq. 4-4 for at least one i.

In addition to being irreducibly diagonally dominant, the $[S]$ matrix should satisfy the conditions:

iii. $a_{i,j} \leq 0$ for all $i \neq j$;

and iv. $a_{i,i} > 0$ for all $1 \leq i \leq n$.

When all the four conditions are satisfied, then $[S]^{-1} > 0$ which means $[S]$ is non-singular. These are the necessary and sufficient conditions to be satisfied by the $[S]$ matrix of Eq. 4-1 to obtain a stable and convergent solution.

According to Strang (1970) there are two kinds of stability to be considered. The first kind depends on the data and the second kind of instability is numerical.

Stability due to data: The stability dependent on the data is equivalent to convergence and this is what Guymon (1970) shows as an empirical factor in his convergence analysis. For the two-dimensional problems solved he assumed the convergence parameter as $\sqrt{A}\,(u + v)/(D_{xx} + D_{yy})$ where A is the area of the triangular finite element. Referring to Fig. 3 (page 79) of Guymon (1970) it appears that when the value of the convergence parameter is less than or equal to about 0.2 the numerical solutions are comparable to the analytic solutions. Guymon (1970) used values for u and v equal to 0.1 mile/year and the longitudinal dispersion coefficient D_L equivalent to about 470 cm^2/sec (0.5656 sq. miles/year).

If D_L is less than 470 cm^2/sec, say about 1.0 cm^2/sec, and $u = v = 0.1$ mile/year, the convergence parameter required is about 167 for the size of the finite elements for the problem shown in Fig. 4-1 and Fig. 4-2. The resulting $[S]$ and $[S]^{-1}$ matrices and the unstable numerical solutions for this problem are given in Appendix H.

On the other hand, for the above problem if the value of $D_L = 1.0$ cm^2/sec and $u = v = 0.1$ mile/year, to obtain a convergence parameter = 0.2, the area A of the triangular finite element should be about 0.00000576 sq. mile which is a negligibly small quantity.

Guymon's empirical relationship for the convergence parameter cannot be used for the new functional because the dispersion coefficients, Eq. 3-2, are not compatible.

In light of Varga's (1962) stability criteria and the fact that Guymon's (1970) convergence parameter developed empirically will not work in the present study, it was decided to consider the whole system of simultaneous first order differential equations represented by Eqs. 3-23 and 3-25 for stability analysis. The elements of the $[S^*]$ matrix of Eq. 3-23 are functions of the finite element network, node numbering, dispersion coefficients and velocity components. Elements of the $[P^*]$ matrix are functions of the finite element network and node numbering only. See Appendix D, Eqs. D-23 and D-24 for development of these matrices.

For a given network of finite elements and node numbering, the elements of the $[P^*]$ matrix of Eq. 3-23 are constants and elements of the $[S^*]$ matrix depend upon the dispersion coefficients D_{xx}, D_{yy}, and D_{xy}, and the velocity components u and v. In addition, when the velocity is steady, u and v are constants and therefore the elements of the $[S^*]$ matrix of Eq. 3-23 depend only upon the dispersion coefficients. In a two-dimensional case, when the velocity components u and v respectively in the x and y directions are equal, Eq. 3-2 reduces to:

$$D_{xx} = D_{yy} = \frac{D_L}{2} + \frac{D_T}{2} + D_d T$$

and

$$D_{xy} = \left(\frac{D_L - D_T}{2}\right) \tag{4-5}$$

If D_T/D_L is taken as a fixed ratio, say 1/10, then $D_T = 0.1\ D_L$ and Eq. 4-5 may be written as:

$$D_{xx} = D_{yy} = 0.55\ D_L + D_d T$$

and

$$D_{xy} = 0.45\ D_L\ . \tag{4-6}$$

Eq. 4-6 shows that D_{xx} and D_{yy} depend upon D_L and D_d for a constant value of the tortuosity factor T and D_{xy} depends upon D_L only.

Normally for liquids the magnitude of the molecular diffusion coefficient D_d is very small and the tortuosity factor is approximately equal to 0.5. The product of D_d and T will be negligible for flow of liquids in porous media. The effect, if any, of the molecular diffusion coefficient D_d on the parameters D_{xx} and D_{yy} is only to increase the magnitudes of these by a very small constant. Instead of using a small value for D_d, the same purpose may be achieved by suitably increasing the value of the longitudinal dispersion coefficient D_L. The expressions for the dispersion coefficients (Eq. 3-2), however, have the advantage of accounting for the molecular diffusion even when the velocity components u and v are both equal to zero. The stability of the final system of equations (Eq. 3-25) to be solved depends upon the longitudinal dispersion coefficient D_L.

An investigation of the properties of the [P] and [S] matrices of Eq. 3-25 for some of the problems solved in this study was undertaken. The [P] matrix satisfied all the necessary conditions developed earlier. The [S] matrix satisfied all the conditions except $a_{i,j} \leq 0$ for all $i \neq j$, which was only approximately satisfied. By this it is meant that for some off-diagonal entries in the [S] matrix $a_{i,j} \approx 0$ (negligibly small positive values). For example, when $D_L = 470\ cm^2/sec$ the values of the elements $a_{3,4}$, $a_{4,3}$, $a_{4,5}$ and $a_{5,4}$ of the [S] matrix for the problem shown in Figs. 4-1 and 4-2 are equal to 0.00208. The numerical solutions for these problems, however, were comparable to the analytic solutions as shown in Table I.

For the same problem, a lower value for the longitudinal dispersion coefficient $D_L = 1.0\ cm^2/sec$ was used keeping all other conditions the same. This resulted in a different [S] matrix and the properties of the matrix changed considerably. For example, $[S]^{-1} \not> 0$ and the condition that $a_{i,j} \leq 0$ for all $i \neq j$ was not satisfied. In fact, $a_{i,j} \geq 0$ for all $i \neq j$. The numerical solution was highly unstable. The [S] and $[S]^{-1}$ matrices and the results obtained are given in Appendix H.

The example problems in the previous paragraphs indicate that Varga's (1962) stability criteria need not be strictly satisfied for obtaining stable solutions in some cases. It appears that in such problems it is possible to obtain stable solutions when only some of the sufficient conditions are satisfied. For example, when Eq. 3-23 is modified for the geometric boundary conditions, the rows corresponding to the boundary condition nodes are eliminated from the system and the column matrix $\{Q^*\}$ on the righthand side of Eq. 3-23 is modified to $\{Q\}$ as in Eq. 3-25. If there are no sources or sinks within the region R, the solution appears to be stable when all the elements of this column matrix $\{Q\}$ are ≥ 0. This happens for each row when the sum of the products of the concentrations at the geometric boundary condition nodes, ϕ_k, $k = 1, 2, \ldots, L$, and the corresponding off-diagonal elements of the $[S^*]$ matrix of Eq. 3-23 is negative at the starting time, i.e.,

$$\sum_{k=1}^{L} a_{i,k}\, \phi_k < 0 \tag{4-7}$$

for all i values $(1 \leq i \leq N-L)$ other than the rows corresponding to the geometric boundary condition nodes. In the types of problems solved in this study, it appears that Eq. 4-7 is a sufficient condition for obtaining stable solutions. For other types of problems such as slug injection, other sufficient conditions could be developed for obtaining stable solutions.

These investigations revealed that care should be exercised in selecting proper sizes and layout of the triangular finite elements, dispersion coefficients and velocity components, and it is suggested that the properties of the matrices $[S]$ and $[P]$ of Eq. 3-25 be evaluated before starting the numerical solution. For field problems, normally the seepage velocity depends upon the hydraulic head, and the dispersion coefficients depend upon the seepage velocity and the dispersivity which is a property of the porous medium. In a given problem with constant velocity distribution the only opportunity that we have is to choose the shape and size of the triangular elements so that the matrices $[S]$ and $[P]$ of Eq. 3-25 satisfy the requirements for obtaining a stable and convergent solution.

Usually in the finite difference method the grids are either square or rectangular. The stability of the system is specified by the size of any one grid. In the finite element method the shape and size of the triangles are chosen arbitrarily. Therefore, the stability of the system cannot be specified with reference to the size of any one triangle and hence the necessity to consider the stability of the whole system of equations, Eq. 3-25.

<u>Stability for unsteady flow</u>: For a given finite element network and node numbering, the $[S]$ matrix in Eq. 3-25 will be different for each time step when the flow is unsteady. The $[S]$ matrix should satisfy the stability requirements discussed in this section for each time step.

<u>Numerical stability</u>: The numerical instability is concerned with the growth of roundoff error. Strang (1970) states that this type of instability is governed by the condition of the equations to be solved

and by the precise algoirthms which are used for the solution. It is suggested that one should use an integrating algorithm which is strongly stable and convergent to minimize numerical instability.

An attempt was made in this study to minimize the numerical instability by using double precision and also by automatically controlling the time step size.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

A method has been developed for predicting the concentration of a dispersing contaminant in a two-dimensional flow field. By discretizing the space variables of the governing partial differential equation using the finite element method and leaving the time variable continuous, the resulting set of linear, first order, ordinary differential equations was numerically solved for the concentrations at a discrete number of points in space. Stability criteria were developed for the resulting matrix set of ordinary differential equations.

5.1 Evaluation of the method and conclusions:

The general partial differential equation for describing the transient concentration distribution in a two-dimensional flow field includes the mixed partial derivatives when the dispersion coefficients are treated as a second order, symmetric tensor. A new functional, Eq. 3-11, was developed based on variational principles to include the mixed partial derivatives which were neglected by previous investigators. The method can handle both longitudinal and lateral dispersion and molecular diffusion if it is significant. The numerical simulator developed by the finite element method can handle irregular boundary shapes very easily.

The results from the numerical simulator compared favorably with the analytic solutions. The results from the problems studied indicate that changes in the data can be easily incorporated in the method. Because of the particular types of boundary conditions incorporated in the functional, a procedure was adopted for one problem using the principles of the method of images to modify the analytic solutions for handling the time dependent boundary conditions. The simulator was also used to solve one approximate case of a non-uniform flow problem and the results appear to agree with the solutions for a similar problem in which the uniform velocity distribution was equal to the average of the velocities in the non-uniform flow case.

The stability criteria requires, that for various input data and finite element network, the $[S]$ and $[P]$ matrices of the resulting set of simultaneous, linear, first-order ordinary differential equations (Eq. 3-25) should satisfy the following sufficient conditions. The $[P]$ matrix should be non-singular and diagonally dominant with positive diagonal entries. The n x n matrix $[S] = (a_{i,j})$ should be non-singular, irreducibly diagonally dominant with $a_{i,j} \leq 0$ for all $i \neq j$, $a_{i,i} > 0$ for all $1 \leq i \leq n$ and $[S]^{-1} > 0$.

One of the advantages of the finite element method is that arbitrary shapes and sizes of triangles can be used within the limitations of the stability requirements discussed earlier. The property of the matrices of the resulting system of equations will depend, in addition to other data, upon the shapes and sizes of the triangular elements. The evaluation of the properties of the matrices is an important aspect before proceeding with the numerical solutions.

5.2 Recommendations for future work:

The assumptions made, the techniques adopted and the results obtained in this research showed that there are several aspects of the problem which require further study. The following recommendations are made for possible future work:

i. It was assumed in Chapter III, for purposes of minimization of the functional, that the concentration varies linearly with respect to the coordinates x and y (Eq. 3-17) over the triangular element. Higher order polynomials could be investigated to see if they improve the solution.

ii. The properties of the resulting system of first order, linear ordinary differential equations may be more thoroughly investigated with regard to stability. The experience gained in this study shows that the type of data used appear to control to a large extent the stability of the system. It may be useful to investigate which of the following data has major influence in controlling the stability of the system: dispersion coefficient, size and shape of the grids, or velocity components.

iii. A method needs to be developed to handle boundary conditions other than those considered in this work, namely natural or reflective boundary conditions and geometric or time invariant boundary conditions.

iv. Different numerical methods for solving the system of ordinary differential equations should be evaluated for computer time requirements and accuracy.

v. Comparison of solutions of the dispersion equation by the finite element method and the finite difference method are needed to define computer storage requirements, computer time and accuracy of the results.

vi. The numerical simulator should be applied to solve a two-dimensional field problem wherein the flow may be unsteady and non-uniform.

vii. As suggested in Appendix C, the functional developed in this study may be utilized to solve the two-dimensional ground water flow equation treating the transmissibility as a symmetric tensor.

REFERENCES

Bachmat, Y. and Jacob Bear. 1964. The general equations of hydrodynamic dispersion in homogeneous, isotropic porous mediums. Journal of Geophysical Research, vol. 69, no. 12, June 15, 1964. pp. 2561-2567.

Bear, Jacob. 1961a. On the tensor form of dispersion in porous media. Journal of Geophysical Research, vol. 66, no. 4, April 1961. pp. 1185-1198.

Bear, Jacob. 1961b. Some experiments in dispersion. Journal of Geophysical Research, vol. 66, no. 8, August 1961. pp. 2455-2467.

Bear, Jacob, D. Zaslavsky and S. Irmay. 1968. Physical principles of water percolation and seepage. United Nations Educational, Scientific and Cultural Organization, vol. XXIX in the series on Arid Zone Research, New York, 1968. 465p.

Bittinger, M. W., H. R. Duke, and R. A. Longenbaugh. 1967. Mathematical simulations for better aquifer management. International Association of Scientific Hydrology, Publication No. 72, Symposium of Haifa, March 1967. pp. 509-519.

Bruch, Jr., John C. 1970. Two dimensional dispersion experiments in a porous medium. Water Resources Research, vol. 6, no. 3, June 1970. pp. 791-800.

Brutsaert, Willem. 1970. Immiscible multiphase flow in ground water hydrology: A computer analysis of the well flow problem. Ph.D. dissertation, Colorado State University, Fort Collins, May 1970.

Carslaw, H. S. and J. C. Jaeger. 1959. Conduction of heat in solids. Oxford University Press, London, 2nd edition, 1959. 510p.

Conte, S. D. 1965. Elementary numerical analysis. McGraw Hill, New York, 1st edition, 1965. 272p.

Crank, J. 1956. The mathematics of diffusion. Oxford University Press, London, 1956. 347p.

de Josselin de Jong, G. 1958. Longitudinal and transverse diffusion in granular deposits. Transactions, American Geophysical Union, vol. 39, no. 1, February 1958. pp. 67-74.

de Josselin de Jong, G. and M. J. Bossen. 1961. Discussion of a paper by Jacob Bear, On the tensor form of dispersion in porous media, Journal of Geophysical Research, vol. 66, no. 10, October 1961. pp. 3623-3624.

De Wiest, R. M. (Editor). 1969. Flow through porous media. Academic Press, New York, 1st edition, 1969. 530p.

Ebach, E. A. and R. R. White. 1958. Mixing of fluids flowing through beds of packed solids. American Institute of Chemical Engineers Journal, vol. 4, no. 2, June 1958. pp. 161-169.

France, P. W., C. J. Parekh, J. C. Peters and C. Taylor. 1971. Numerical analysis of free surface seepage problems. Proceedings, American Society of Civil Engineers (Irrigation and Drainage Division), vol. 97, IR1, Paper No. 7959, March 1971. pp. 165-179.

Garder, A. O., D. W. Peaceman and A. L.Pozzi, Jr. 1964. Numerical calculation of multidimensional miscible displacement by the method of characteristics. Society of Petroleum Engineers Journal, vol. 4, no. 1, March 1964. pp. 26-36.

Guymon, L. R. Gary. 1970. Mathematical modelling of movement of dissolved constituents in ground water aquifers by the finite element method. Ph.D. dissertation, University of California, Davis, January 1970. 99p.

Guymon, G. L., V. H. Scott, and L. R. Herrmann. 1970. A general numerical solution of the two-dimensional diffusion convection equation by the finite element method. Water Resources Research, vol. 6, no. 6, December 1970. pp. 1611-1617.

Harleman, D. R. F. and R. R. Rumer, Jr. 1963. Longitudinal and lateral dispersion in an isotropic porous medium. Journal of Fluid Mechanics, vol. 16, Part 3, July 1963. pp. 385-394.

Harleman, D. R. F., P. F. Mehlhorn and R. R. Rumer, Jr. 1963. Dispersion-permeability correlation in porous media. Proceedings, American Society of Civil Engineers (Hydraulics Division), vol. 89, HY2, Paper No. 3459, March 1963. pp. 67-85.

Hildebrand, F. B. 1965. Methods of applied mathematics. Prentice-Hall, Inc., New Jersey, 2nd edition, 1965. 362p.

Hoopes, J. A. and D. R. F. Harleman. 1965. Waste water recharge and dispersion in porous media. Technical Report No. 75, Hydrodynamics Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts, June 1965. 166p.

Javandel, Iraj, and P. A. Witherspoon. 1968. Application of the finite element method to transient flow in porous media. Society of Petroleum Engineers Journal, vol. 8, no. 3, September 1968. pp. 241-252.

Javandel, I., and P. A. Witherspoon. 1968a. Analysis of transient fluid flow in multi-layered systems. Water Resources Center Contribution No. 124, University of California, Berkeley, 1968. 119p.

Javandel, Iraj and Paul A. Witherspoon. 1969. A method of analysing transient fluid flow in multilayered aquifers. Water Resources Research, vol. 5, no. 4, August 1969. pp. 856-869.

Neuman, P. Solomon and Paul A. Witherspoon. 1970a. Finite element method of analysing steady seepage with a free surface. Water Resources Research, vol. 6, no. 3, June 1970. pp. 889-897.

Neuman, P. Solomon and Paul A. Witherspoon. 1970b. Variational principles for confined and unconfined flow of ground water. Water Resources Research, vol. 6, no. 5, October 1970. pp. 1376-1382.

Ogata, A. and R. B. Banks. 1961. A solution of the differential equation of longitudinal dispersion in porous media. Professional Paper 411-A, U. S. Geological Survey, U. S. Govt. Printing Office, Washington, D. C. 7p.

Peaceman, D. W. and H. H. Rachford, Jr. 1962. Numerical calculation of multidimensional miscible displacement. Society of Petroleum Engineers Journal, vol. 2, no. 4, December 1962. pp. 327-339.

Pinder, G. F. and H. H. Cooper, Jr. 1970. A numerical technique for calculating the transient position of the salt water front. Water Resources Research, vol. 6, no. 3, June 1970. pp. 875-882.

Pinder, G. F. and J. D. Bredehoeft. 1968. Application of the digital computer for aquifer evaluation. Water Resources Research, vol. 4, no. 5, October 1968. pp. 1069-1093.

Reddell, D. L. 1969. Dispersion in ground water flow systems. Ph. D. dissertation, Colorado State University, Fort Collins, December 1969. 117p.

Reddell, D. L. and D. K. Sunada. 1970. Numerical simulation of dispersion in ground water aquifers. Hydrology Paper No. 41, Colorado State University, Fort Collins, June 1970. 79p.

Sandhu, S. Ranbir. 1969. Finite element analysis of seepage in elastic media. Proceedings, American Society of Civil Engineers (Engineering Mechanics Division), vol. 95, EM3, Paper No. 6615, June 1969. pp. 641-652.

Schechter, R. S. 1967. The variational method in engineering. McGraw-Hill,New York, 1st edition, 1967. 287p.

Scheidegger, A. E. 1961. General theory of dispersion in porous media. Journal of Geophysical Research, vol. 66, no. 10, October 1961. pp. 3273-3278.

Shamir, U. Y. and D. R. F. Harleman. 1967. Numerical solutions for dispersion in porous mediums. Water Resources Research, vol. 3, no. 2, 2nd quarter 1967. pp. 557-581.

Strang, Gilbert. 1970. The finite element method and approximation theory. Paper presented for the Symposium on the numerical solution of partial differential equations at the University of Maryland in May 1970.

Taylor, G. I. 1953. Dispersion of soluble matter in solvent flowing slowly through a tube. Proceedings, Royal Society of London, Series A, vol. 219, pp. 186-203.

Taylor, G. I. 1954. The dispersion of matter in turbulent flow through a pipe. Proceedings, Royal Society of London, Series A, vol. 223. pp. 446-468.

Taylor, R. L. and C. B. Brown. 1967. Darcy flow solutions with a free surface. Proceedings, American Society of Civil Engineers (Hydraulics Division), vol. 93, HY2, Paper No. 5126, March 1967. pp. 25-38.

Todorovic, P. 1970. A stochastic model of longitudinal diffusion in porous media. Water Resources Research, vol. 6, no. 1, February 1970. pp. 211-222.

Tyson, Jr. N. H. and E. M. Weber. 1964. Ground water management for the nation's future - computer simulation of ground water basins. Proceedings, American Society of Civil Engineers (Hydraulics Division), vol. 90, HY4, Paper No. 3973, July 1964. pp. 59-77.

U. S. Army Corps of Engineers. 1970. Finite element solution of steady state potential flow problems, generalized computer program, 723-440. The Hydrologic Engineering Center, Davis, California, November 1970. 48p.

Varga, Richard S. 1962. Matrix iterative analysis. Prentice-Hall, Inc., New Jersey, 1st edition, 1962. 322p.

Wilson, E. L. and R. E. Nickell. 1966. Application of the finite element method to heat conduction analysis. Nuclear Engineering and Design, 4(1966). pp. 276-286.

Witherspoon, Paul A., I. Javandel and S. P. Neuman. 1968. Use of the finite element method in solving transient flow problems in aquifer systems. University of Arizona symposium in the use of analog and digital computers in hydrology, 1968.

Zienkiewicz, O. C. and Y. K. Cheung. 1965. Finite elements in the solution of field problems. The Engineer, vol. 220, September 1965. pp. 507-510.

Zienkiewicz, O. C. and Y. K. Cheung. 1967. The finite element method in structural and continuum mechanics. McGraw-Hill, London, 1967. 272p.

Zienkiewicz, O. C., P. Mayer and Y. K. Cheung. 1966. Solution of anisotropic seepage by finite elements. Proceedings, American Society of Civil Engineers (Engineering Mechanics Division), vol. 92, EM1, Paper No. 4676, February 1966. pp. 111-120.

APPENDICES

APPENDIX A

DISPERSION EQUATION IN ROTATED COORDINATE SYSTEM

Eq. 3-3 represents the mathematical model describing the transient concentration distribution in a two-dimensional Cartesian coordinate system x and y. Let x' and y' be another set of orthogonal Cartesian coordinates rotated through an angle θ with respect to the coordinates x and y as shown in Fig. A-1. The relationships between the two systems are given by

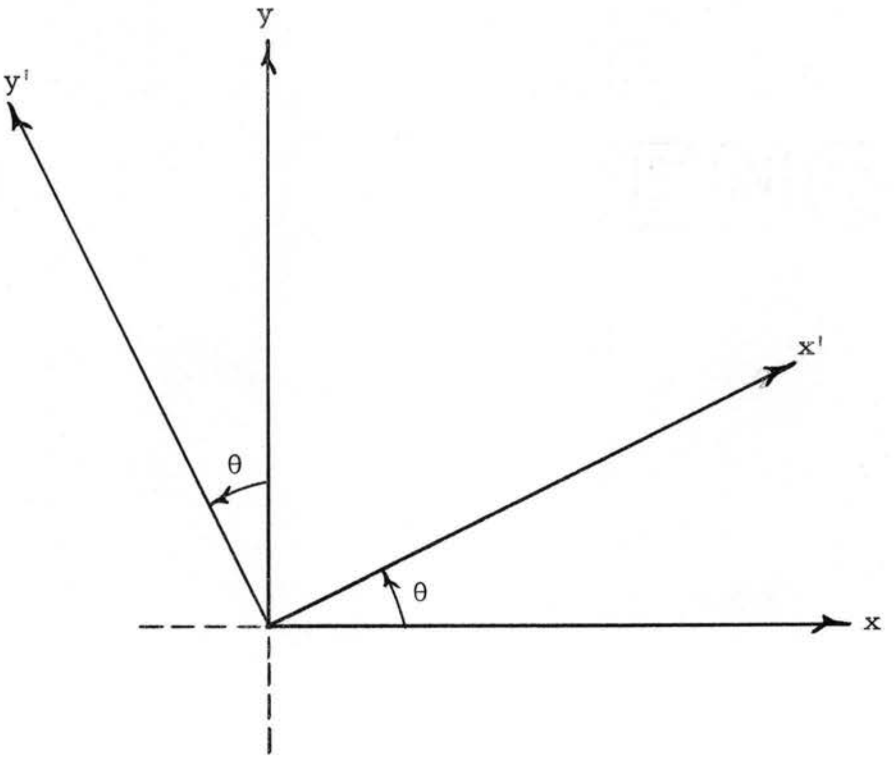


Fig. A-1 Two-dimensional rotation of axes.

$$x' = x \cos\theta + y \sin\theta$$
$$\text{and} \quad y' = -x \sin\theta + y \cos\theta \,. \tag{A-1}$$

The rotation matrix is

$$\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \tag{A-2}$$

which transforms the dispersion matrix

$$\begin{bmatrix} D_{xx} & D_{xy} \\ D_{xy} & D_{yy} \end{bmatrix} \tag{A-3}$$

into a diagonal matrix

$$\begin{bmatrix} D_{x'x'} & 0 \\ 0 & D_{y'y'} \end{bmatrix} \tag{A-4}$$

$$\text{where} \quad D_{x'x'} = D_{xx} \operatorname{Cos}^2\theta + 2\, D_{xy} \operatorname{Sin}\theta \operatorname{Cos}\theta + D_{yy} \operatorname{Sin}^2\theta$$
$$\text{and} \quad D_{y'y'} = D_{xx} \operatorname{Sin}^2\theta - 2D_{xy} \operatorname{Sin}\theta \operatorname{Cos}\theta + D_{yy} \operatorname{Cos}^2\theta \tag{A-5}$$

Similarly, the rotation matrix, Eq. A-2, transforms the convective terms u and v in xy coordinate system into the corresponding terms in $x'y'$ coordinates as

$$u' = u \operatorname{Cos}\theta + v \operatorname{Sin}\theta$$
$$\text{and} \quad v' = -u \operatorname{Sin}\theta + v \operatorname{Cos}\theta \,. \tag{A-6}$$

APPENDIX B

MATHEMATICAL DEVELOPMENTS

<u>Derivation of the reducing factor exp (β) in Eq. 3-9</u>: Eq. 3-3 may be written as

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + 2D_{xy}\frac{\partial^2 C}{\partial x \partial y} + D_{yy}\frac{\partial^2 C}{\partial y^2} - u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - \frac{\partial C}{\partial t} = 0 \tag{B-1}$$

It may be assumed that the dispersion coefficients and the velocity components in Eq. B-1 are constants over the area of a triangular finite element. If $A = A(x, y)$ is assumed as the reducing factor, then according to Hildebrand (1965) the reducing factor must satisfy the simultaneous, first order partial differential equations

$$D_{xx}\frac{\partial A}{\partial x} + D_{xy}\frac{\partial A}{\partial y} = -u\,A \tag{B-2}$$

$$D_{xy}\frac{\partial A}{\partial x} + D_{yy}\frac{\partial A}{\partial y} = -v\,A\ . \tag{B-3}$$

Eqs. B-2 and B-3 can be solved simultaneously to obtain

$$\frac{\partial A}{\partial x} = \left(\frac{-u\,D_{yy} + v\,D_{xy}}{-v\,D_{xx} + u\,D_{xy}}\right)\frac{\partial A}{\partial y}\quad . \tag{B-4}$$

Using the method of separation of variables, it can be proven that the reducing factor

$$A = \exp\ (\beta) \tag{B-5}$$

$$\text{where} \quad \beta = \left(\frac{D_{xy}\, v - D_{yy}\, u}{D_{xx}\, D_{yy} - D_{xy}^2}\right) x + \left(\frac{D_{xy}\, u - D_{xx}\, v}{D_{xx}\, D_{yy} - D_{xy}^2}\right) y\ . \tag{B-6}$$

The expression for β , Eq. B-6, may be modified using Eq. 3-2 for the dispersion coefficients to avoid zero in the denominator. The modified form is

$$\beta = -\left(\frac{u\, x + v\, y}{D_L + D_d T}\right) \tag{B-7}$$

Eq. B-7 is equivalent to Eq. 3-10.

Proof of equivalence of the functional and the differential equation: The functional given by Eq. 3-11 is proved to be equivalent to the differential equation given by Eq. 3-3 with boundary conditions, Eqs. 3-4 and 3-5. Given the functional, Eq. 3-11,

$$J = \iint_R \exp\ (\beta) \left\{ \frac{1}{2} \left[D_{xx} \left(\frac{\partial C}{\partial x}\right)^2 + 2\, D_{xy} \left(\frac{\partial C}{\partial x}\right)\left(\frac{\partial C}{\partial y}\right) + D_{yy}\left(\frac{\partial C}{\partial y}\right)^2 \right] + \left(\frac{\partial C}{\partial t}\right) C \right\} dx\, dy \tag{B-8}$$

where β , D_{xx} , D_{xy} and D_{yy} are applicable to the region R (Fig. 3-1), a small variation of the functional may be taken utilising the variational principles and assuming $\frac{\partial C}{\partial t}$ as invariant at any instant of time, and equated to zero.

$$\delta J = \iint_R \exp(\beta)\Big[D_{xx}\left(\frac{\partial C}{\partial x}\right)\frac{\partial}{\partial x}(\delta C) + D_{xy}\left(\frac{\partial C}{\partial x}\right)\frac{\partial}{\partial y}(\delta C)$$

$$+ D_{xy}\left(\frac{\partial C}{\partial y}\right)\frac{\partial}{\partial x}(\delta C) + D_{yy}\left(\frac{\partial C}{\partial y}\right)\frac{\partial}{\partial y}(\delta C) + \left(\frac{\partial C}{\partial t}\right)\delta C\Big]\, dxdy = 0$$

(B-9)

Using integration by parts and Green's theorem Eq. B-9 may be written as

$$\delta J = \int_\Gamma \exp(\beta)\left[\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right)dy + \left(D_{xy}\frac{\partial C}{\partial x} + D_{yy}\frac{\partial C}{\partial y}\right)dx\right]\delta C$$

$$- \iint_R \Big[\frac{\partial}{\partial x}\left(\exp(\beta) D_{xx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\exp(\beta) D_{xy}\frac{\partial C}{\partial x}\right)$$

$$+ \frac{\partial}{\partial x}\left(\exp(\beta) D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(\exp(\beta) D_{yy}\frac{\partial C}{\partial y}\right) - \exp(\beta)\frac{\partial C}{\partial t}\Big]\delta C\, dxdy = 0$$

(B-10)

where Γ is the boundary of the region R.

Applying the fundamental lemma of the calculus of variations to the area integral of Eq. B-10 yields

$$\frac{\partial}{\partial x}\left[\exp(\beta) D_{xx}\frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial y}\left[\exp(\beta) D_{xy}\frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial x}\left[\exp(\beta) D_{xy}\frac{\partial C}{\partial y}\right]$$

$$+ \frac{\partial}{\partial y}\left[\exp(\beta) D_{yy}\frac{\partial C}{\partial y}\right] - \exp(\beta)\frac{\partial C}{\partial t} = 0 \qquad \text{(B-11)}$$

Expanding the above and grouping the terms and dividing out the exponential terms, the following partial differential equation is obtained which is equivalent to Eq. 3-3:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_{xx}\frac{\partial^2 C}{\partial x^2} + 2\,D_{xy}\frac{\partial^2 C}{\partial x \partial y} + D_{yy}\frac{\partial^2 C}{\partial y^2}$$

(B-12)

The line integral in Eq. B-10 is to be integrated along the boundary of the region R in Fig. 3-1. On the portion of the boundary where the concentration is fixed (Eq. 3-4) $\delta C = 0$ and therefore the line integral is zero. On the remaining portion of the boundary, the concentration gradient in the outward normal direction $\frac{\partial C}{\partial n} = 0$ corresponding to Eq. 3-5. This means that the dispersive flux across the boundary is zero, Reddell and Sunada (1970). This is equivalent to making the integrand of the line integral, namely

$$\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) = 0 \quad \text{and} \quad \left(D_{xy}\frac{\partial C}{\partial x} + D_{yy}\frac{\partial C}{\partial y}\right) = 0$$

(B-13)

Therefore, for both types of boundary conditions considered, the line integral

$$\int_{\Gamma} \exp(\beta)\left[\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right)dy + \left(D_{xy}\frac{\partial C}{\partial x} + D_{yy}\frac{\partial C}{\partial y}\right)dx\right]\delta C = 0$$

(B-14)

Thus the functional, Eq. 3-11, is equivalent to the differential Eq. 3-3 and the boundary conditions, Eqs. 3-4 and 3-5.

<u>Proof of equivalence of the functional, Eq. 3-16, and the differential Eq. 3-13:</u> In this section the functional given by Eq. 3-16 is proved to be equivalent to the differential equation in terms of the transformed value of the concentration ϕ (Eq. 3-13) with boundary conditions, Eqs. 3-14 and 3-15. The functional in terms of the transformed value of the concentration ϕ is:

$$J = \iint_R \left\{ \frac{D_{xx}}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + D_{xy}\left(\frac{\partial\phi}{\partial x}\right)\left(\frac{\partial\phi}{\partial y}\right) + \frac{D_{yy}}{2}\left(\frac{\partial\phi}{\partial y}\right)^2 + \left(\frac{u}{2}\frac{\partial\phi}{\partial x} + \frac{v}{2}\frac{\partial\phi}{\partial y}\right)\phi \right.$$

$$\left. + \left[\frac{D_{yy}u^2 + D_{xx}v^2 - 2D_{xy}uv}{8(D_{xx}D_{yy} - D_{xy}^2)}\right]\phi^2 + \left(\frac{\partial\phi}{\partial t}\right)\phi \right\} dx\,dy \tag{B-15}$$

where the dispersion coefficients and the velocity components are applicable to the region R (Fig. 3-1). Assuming $\left(\frac{\partial\phi}{\partial t}\right)$ as invariant at any particular instant of time and utilising the variational principles a small variation of the functional is taken and equated to zero.

$$\delta J = \iint_R \left\{ D_{xx}\left(\frac{\partial\phi}{\partial x}\right)\frac{\partial}{\partial x}(\delta\phi) + D_{xy}\left(\frac{\partial\phi}{\partial x}\right)\frac{\partial}{\partial y}(\delta\phi) + D_{xy}\frac{\partial\phi}{\partial y}\frac{\partial}{\partial x}(\delta\phi) \right.$$

$$+ D_{yy}\left(\frac{\partial\phi}{\partial y}\right)\frac{\partial}{\partial y}(\delta\phi) + \left(\frac{u}{2}\frac{\partial\phi}{\partial x} + \frac{v}{2}\frac{\partial\phi}{\partial y}\right)\delta\phi$$

$$+ \left(\frac{u}{2}\frac{\partial(\delta\phi)}{\partial x} + \frac{v}{2}\frac{\partial(\delta\phi)}{\partial y}\right)\phi + \left[\frac{D_{yy}u^2 + D_{xx}v^2 - 2D_{xy}uv}{4(D_{xx}D_{yy} - D_{xy}^2)}\right]\phi\delta\phi$$

$$\left. + \left(\frac{\partial\phi}{\partial t}\right)\delta\phi \right\} dx\,dy = 0 \tag{B-16}$$

Using integration by parts and Green's theorem, we get,

$$\delta J = \int_\Gamma \left[\left(D_{xx}\frac{\partial\phi}{\partial x} + D_{xy}\frac{\partial\phi}{\partial y}\right) dy + \left(D_{yy}\frac{\partial\phi}{\partial y} + D_{xy}\frac{\partial\phi}{\partial x}\right) dx\right] \delta\phi$$

$$+ \int_\Gamma \left(\frac{u}{2}\ \phi\, dy + \frac{v}{2}\ \phi\, dx\right) \delta\phi$$

$$- \iint_R \left\{\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{xy}\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{xy}\frac{\partial\phi}{\partial y}\right)\right.$$

$$+ \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial\phi}{\partial y}\right) - \left(\frac{u}{2}\ \frac{\partial\phi}{\partial x} + \frac{v}{2}\ \frac{\partial\phi}{\partial y}\right)$$

$$+ \frac{\partial}{\partial x}\left(\frac{u}{2}\ \phi\right) + \frac{\partial}{\partial y}\left(\frac{v}{2}\ \phi\right) - \left[\frac{D_{yy}u^2 + D_{xx}v^2 - 2D_{xy}uv}{4(D_{xx}D_{yy} - D_{xy}^2)}\right]\phi$$

$$\left. - \left(\frac{\partial\phi}{\partial t}\right)\right\} \delta\,\phi\, dx\, dy = 0 \qquad \text{(B-17)}$$

Applying the fundamental lemma of the calculus of variations to the area integral in Eq. B-17 yields

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{xy}\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{xy}\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial\phi}{\partial y}\right)$$

$$- \left[\frac{D_{yy}u^2 + D_{xx}v^2 - 2D_{xy}u\,v}{4(D_{xx}D_{yy} - D_{xy}^2)}\right]\phi - \left(\frac{\partial\phi}{\partial t}\right) = 0 \qquad \text{(B-18)}$$

Assuming the dispersion coefficients as constants, we have,

$$\frac{\partial \phi}{\partial t} + \left[\frac{D_{yy} u^2 + D_{xx} v^2 - 2 D_{xy} u v}{4(D_{xx} D_{yy} - D_{xy}^2)} \right] \phi$$

$$= D_{xx} \frac{\partial^2 \phi}{\partial x^2} + 2 D_{xy} \frac{\partial^2 \phi}{\partial x \partial y} + D_{yy} \frac{\partial^2 \phi}{\partial y^2} . \qquad \text{(B-19)}$$

Eq. B-19 is the same as Eq. 3-13.

The line integral in Eq. B-17

$$\int_{\Gamma} \left[\left(D_{xx} \frac{\partial \phi}{\partial x} + D_{xy} \frac{\partial \phi}{\partial y} + u \frac{\phi}{2} \right) d\,y + \left(D_{yy} \frac{\partial \phi}{\partial y} + D_{xy} \frac{\partial \phi}{\partial x} + v \frac{\phi}{2} \right) dx \right] \delta\phi$$

$$\text{(B-20)}$$

is to be proved to be equal to zero. On the portion of the boundary where the concentration is fixed corresponding to the Eq. 3-14, $\delta\phi = 0$ and therefore the line integral is zero. On the remaining portion of the boundary the quantity within the square brackets in Eq. B-20 should equal zero. This situation corresponds to the natural boundary condition represented by Eq. 3-15. Utilising the relationships of Eq. B-13 it can be proved that for that portion of the boundary where $\delta\phi \neq 0$, the quantity within the square brackets of Eq. B-20 is zero. Therefore, for both types of boundary conditions under consideration (Eqs. 3-14 and 3-15), the line integral is zero. Thus the functional given by Eq. 3-16 is equivalent to the differential Eq. 3-13 with boundary conditions, Eqs. 3-14 and 3-15.

APPENDIX C

METHOD OF SOLVING THE FLOW EQUATION

Extension of the functional for solving the ground water flow equation: The functional given by Eq. 3-11 may be utilized for solving the ground water flow equation, considering the medium as anisotropic and nonhomogeneous with regard to permeability. Zienkiewicz, et. al. (1966) solved by the finite element method anisotropic seepage problem for a steady flow case. Though the permeability was considered as anisotropic, they made use of a transformation to get rid of the anti-symmetrical part of the permeability tensor (skew tensor) thereby reducing the partial differential equation to one without mixed partial derivatives. In the following procedure no such transformation is necessary as the proposed functional includes the effect of the mixed partial derivatives.

The differential equation describing the nonsteady ground water flow in an anisotropic, nonhomogeneous porous medium can be stated as (Pinder and Bredehoeft, 1968):

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial H}{\partial x_j}\right) = S\frac{\partial H}{\partial t} \qquad \text{(C-1)}$$

where T_{ij} = symmetric transmissibility tensor,

H = hydraulic head,

S = storage coefficient,

and i, j = index coordinates.

There is no source or sink term involved in Eq. C-1.

In a two-dimensional case, assuming the medium as anisotropic and nonhomogeneous with regard to permeability, Eq. C-1 can be written (in Cartesian coordinates) as:

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial x}\left(T_{xy}\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial y}\left(T_{yx}\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_{yy}\frac{\partial H}{\partial y}\right)=S\frac{\partial H}{\partial t} \tag{C-2}$$

Assuming the transmissibility as constant over any triangular finite element and using the fact that the transmissibility $T_{xy} = T_{yx}$, Eq. C-2 can be written as:

$$T_{xx}\frac{\partial^2 H}{\partial x^2} + 2T_{xy}\frac{\partial^2 H}{\partial x\,\partial y} + T_{yy}\frac{\partial^2 H}{\partial y^2} = S\frac{\partial H}{\partial t} \tag{C-3}$$

In Eq. 3-3 after substituting the convective terms u and v both equal to zero, if we replace the dependent variable C by the hydraulic head H and the dispersion tensor D_{ij} by the transmissibility tensor T_{ij} and multiply the time derivative $\frac{\partial C}{\partial t}$ by the storage coefficient S, Eq. C-3 results. With the above modifications, the functional (corresponding to the functional given by Eq. 3-11) for Eq. C-3 may be written as:

$$J = \iint_R \left\{\frac{1}{2}\left[T_{xx}\left(\frac{\partial H}{\partial x}\right)^2 + 2T_{xy}\left(\frac{\partial H}{\partial x}\right)\left(\frac{\partial H}{\partial y}\right) + T_{yy}\left(\frac{\partial H}{\partial y}\right)^2\right] + \left(S\frac{\partial H}{\partial t}\right)H\right\} dx\,dy \tag{C-4}$$

because in this case β is zero, and hence the reducing factor $\exp(\beta) = 1$.

Eq. C-3 is general and applicable to a porous medium in a two-dimensional case having anisotropic and nonhomogeneous permeability. The functional given by Eq. C-4 may be used in conjunction with the finite element method to solve for the hydraulic head H in Eq. C-3.

APPENDIX D

FINITE ELEMENT CHARACTERISTICS

Consider a typical triangle i, j, k as shown in Fig. D-1. The concentration at the point (x, y) within the triangular element is given by the linear polynomial (Eq. 3-17) as

$$\phi = \alpha_1 + \alpha_2 x + \alpha_3 y \quad . \tag{D-1}$$

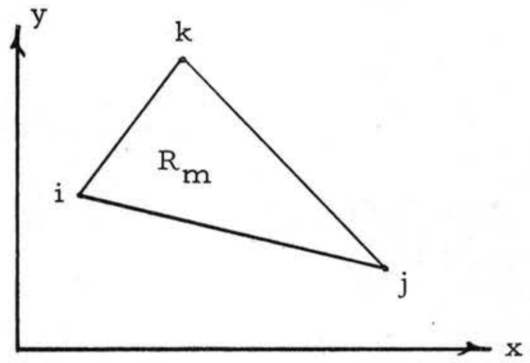


Fig. D-1.

As the plane thus defined has to pass through ϕ_i when $x = x_i$ and $y = y_i$, we have

$$\phi_i = \alpha_1 + \alpha_2 x_i + \alpha_3 y_i$$

similarly, $$\phi_j = \alpha_1 + \alpha_2 x_j + \alpha_3 y_j \tag{D-2}$$

and $$\phi_k = \alpha_1 + \alpha_2 x_k + \alpha_3 y_k \quad .$$

Using Cramer's rule to evaluate the three coefficients α_1, α_2 and α_3 in Eq. D-2 in terms of the coordinates of the nodes and the corresponding nodal values of ϕ we obtain

$$\phi = \frac{1}{2A^m}\left[(a_{1i}+a_{2i}x+a_{3i}y),\ (a_{1j}+a_{2j}x+a_{3j}y),\ (a_{1k}+a_{2k}x+a_{3k}y)\right]\begin{Bmatrix}\phi_i\\ \phi_j\\ \phi_k\end{Bmatrix} \quad \text{(D-3)}$$

where A^m is the area of the m^{th} triangular element,

or simply

$$\phi = \left[A_{(i)},\ A_{(j)},\ A_{(k)}\right]\ \{\phi\}^m \quad \text{(D-4)}$$

in which $\{\phi\}^m$ stands for the values of the concentrations characteristic of the m^{th} element considered. The coefficients in Eq. D-3 are defined as

$$a_{1i} = x_j y_k - x_k y_j ,$$
$$a_{2i} = y_j - y_k \quad \text{(D-5)}$$
$$\text{and} \quad a_{3i} = x_k - x_j$$

with others following a cyclic, anticlockwise order in i, j and k. The row matrix in Eq. D-4 is a function of space only and the column matrix is a function of time only.

In general, ϕ for any particular element m of the system may be written as

$$\phi = \left[A\right]\ \{\phi\}^m \quad \text{(D-6)}$$

where $\left[A\right] = \left[A_{(i)}, \; A_{(j)}, \; A_{(k)}\right]$

and $\quad \{\phi\}^m = \begin{Bmatrix} \phi_i \\ \phi_j \\ \phi_k \end{Bmatrix}$.

Eq. D-6 is equivalent to Eq. 3-20.

The contribution of the i^{th} node of the m^{th} triangular element to the differential of the function J is:

$$\frac{\partial J^m}{\partial \phi_i} = \iint_{R_m} \left\{ D_{xx} \frac{\partial\phi}{\partial \xi} \frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\xi}\right) + D_{xy}\left[\frac{\partial\phi}{\partial\xi}\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\eta}\right) + \frac{\partial\phi}{\partial\eta}\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\xi}\right)\right]\right.$$

$$+ D_{yy}\frac{\partial\phi}{\partial\eta}\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\eta}\right) + \left[\frac{u}{2}\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\xi}\right) + \frac{v}{2}\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\eta}\right)\right]\phi$$

$$+\left[\frac{u}{2}\frac{\partial\phi}{\partial\xi} + \frac{v}{2}\frac{\partial\phi}{\partial\eta}\right]\frac{\partial\phi}{\partial\phi_i}$$

$$\left. + \left[\frac{u^2+v^2}{4(D_L+D_d T)}\right]\phi\frac{\partial\phi}{\partial\phi_i} + \left(\frac{\partial\phi}{\partial t}\right)\frac{\partial\phi}{\partial\phi_i}\right\} d\xi \, d\eta \qquad \text{(D-7)}$$

where R_m denotes the region of the m^{th} triangular element. The various terms in Eq. D-7 are evaluated from Eq. D-6 as follows:

$$\frac{\partial\phi}{\partial t} = \left[A\right]\left\{\frac{\partial\phi}{\partial t}\right\}^m \qquad \text{(D-8)}$$

$$\frac{\partial\phi}{\partial\xi} = \frac{\partial\phi}{\partial x} = \frac{1}{2A^m} \left[a_2\right]\{\phi\}^m \tag{D-9}$$

$$\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\xi}\right) = \frac{1}{2A^m}\left(a_{2i}\right) \tag{D-10}$$

$$\frac{\partial\phi}{\partial\eta} = \frac{\partial\phi}{\partial y} = \frac{1}{2A^m} \left[a_3\right]\{\phi\}^m \tag{D-11}$$

$$\frac{\partial}{\partial\phi_i}\left(\frac{\partial\phi}{\partial\eta}\right) = \frac{1}{2A^m}\left(a_{3i}\right) \tag{D-12}$$

and $$\frac{\partial\phi}{\partial\phi_i} = A_{(i)} = \left[a_{1i} + a_{2i}x + a_{3i}y\right] \Big/ 2A^m \tag{D-13}$$

where
$$\left[a_2\right] = \left[a_{2i}, \; a_{2j}, \; a_{2k}\right]$$
$$\left[a_3\right] = \left[a_{3i}, \; a_{3j}, \; a_{3k}\right]$$
$$\{\phi\}^m = \begin{Bmatrix} \phi_i \\ \phi_j \\ \phi_k \end{Bmatrix} .$$

Using the values from Eqs. D-8 to D-13 in Eq. D-7 we get

$$\frac{\partial J^m}{\partial\phi_i} = \int\int_{R_m}\Bigg\{D_{xx}\left(\frac{1}{2A^m}\left[a_2\right]\{\phi\}^m \frac{a_{2i}}{2A^m}\right)$$

$$+ D_{xy}\left(\frac{1}{2A^m}\left[a_2\right]\{\phi\}^m \frac{a_{3i}}{2A^m} + \frac{1}{2A^m}\left[a_3\right]\{\phi\}^m \frac{a_{2i}}{2A^m}\right)$$

$$+ D_{yy}\left(\frac{1}{2A^m}\left[a_3\right]\{\phi\}^m \frac{a_{3i}}{2A^m}\right)$$

$$+\left[\frac{u}{2}\,\frac{a_{2i}}{2A^m} + \frac{v}{2}\,\frac{a_{3i}}{2A^m}\right]\left[A\right]\{\phi\}^m$$

$$+\left[\frac{u}{2}\,\frac{1}{2A^m}\left[a_2\right]\{\phi\}^m + \frac{v}{2}\,\frac{1}{2A^m}\left[a_3\right]\{\phi\}^m\right] A_{(i)}$$

$$+\left[\frac{u^2+v^2}{4(D_L+D_d T)}\right]\left[A\right]\{\phi\}^m \quad A_{(i)}$$

$$\left. + \quad \left[A\right]\left\{\frac{\partial\phi}{\partial t}\right\}^m \quad A_{(i)}\right\} d\xi \; d\eta \qquad \text{(D-14)}$$

Assuming D_{xx}, D_{yy}, D_{xy}, u and v as constants over a triangular element and using the integration formulas defined in this section (Eqs. D-16 to D-22) in Eq. D-14, we get,

$$\frac{\partial J^m}{\partial \phi_i} = \left\{\left[\frac{D_{xx}}{4A^m}\,a_{2i}\left[a_2\right] + \frac{D_{xy}}{4A^m}\,a_{3i}\left[a_2\right] + \frac{D_{xy}}{4A^m}\,a_{2i}\left[a_3\right] + \frac{D_{yy}}{4A^m}\,a_{3i}\left[a_3\right]\right.\right.$$

$$+ \frac{1}{12}\left(u\,a_{2i} + v\,a_{3i}\right)\left[1, 1, 1\right]$$

$$+ \frac{1}{12}\left(u\left[a_2\right] + v\left[a_3\right]\right)$$

$$\left. + \frac{1}{16A^m}\left(\frac{u^2+v^2}{D_L + D_d T}\right)\left[(AA)_i\right]\right]\{\phi\}^m$$

$$\left. + \frac{\left[(AA)_i\right]}{4A^m}\left\{\frac{\partial\phi}{\partial t}\right\}^m\right\} \qquad \text{(D-15)}$$

Integration formulas: The following relationships are used for deriving Eq. D-15. For a triangle with local coordinates ξ_i, ξ_j, ξ_k, η_i, η_j and η_k, we have

$$\frac{\xi_i + \xi_j + \xi_k}{3} = \frac{\eta_i + \eta_j + \eta_k}{3} = 0$$

1. $$\iint_{R_m} d\xi \, d\eta = \frac{1}{2} \begin{vmatrix} 1 & \xi_i & \eta_i \\ 1 & \xi_j & \eta_j \\ 1 & \xi_k & \eta_k \end{vmatrix} = A^m \qquad \text{(D-16)}$$

2. $$\iint_{R_m} \xi \, d\xi \, d\eta = \iint_{R_m} \eta \, d\xi \, d\eta = 0 \qquad \text{(D-17)}$$

3. $$\iint_{R_m} \xi^2 \, d\xi \, d\eta = \frac{A^m}{12} \left(\xi_i^2 + \xi_j^2 + \xi_k^2 \right) \qquad \text{(D-18)}$$

4. $$\iint_{R_m} \eta^2 \, d\xi \, d\eta = \frac{A^m}{12} \left(\eta_i^2 + \eta_j^2 + \eta_k^2 \right) \qquad \text{(D-19)}$$

5. $$\iint_{R_m} \xi \, \eta \, d\xi \, d\eta = \frac{A^m}{12} \left(\xi_i \eta_i + \xi_j \eta_j + \xi_k \eta_k \right) \qquad \text{(D-20)}$$

6. $$\iint_{R_m} \left[A\right] d\xi \, d\eta = \iint_{R_m} \left[A_{(i)}, A_{(j)}, A_{(k)}\right] d\xi \, d\eta$$

$$= \left[\iint_{R_m} A_{(i)} d\xi \, d\eta, \iint_{R_m} A_{(j)} \, d\xi \, d\eta, \iint_{R_m} A_{(k)} \, d\xi \, d\eta \right]$$

and $$\iint_{R_m} A_{(n)}\, d\xi\, d\eta = \frac{1}{2A^m} \iint_{R_m} \left[a_{1n} + a_{2n}(\xi + \overline{x}) + a_{3n}(\eta + \overline{y})\right] d\xi\, d\eta$$

$$= \frac{1}{2}\left(a_{1n} + a_{2n}\overline{x} + a_{3n}\overline{y}\right)$$

For n = i ,

$$\iint_{R_m} A_{(i)}\, d\xi\, d\eta = \frac{1}{2}\Big[(x_j y_k - x_k y_j) + (y_j - y_k)(x_i + x_j + x_k)\frac{1}{3}$$

$$+ (x_k - x_j)(y_i + y_j + y_k)\frac{1}{3}\Big]$$

$$= \frac{1}{6}\begin{vmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{vmatrix} = \frac{A^m}{3}$$

Similarly for $n = j , k$

$$\iint_{R_m} A_{(n)}\, d\xi\, d\eta = \frac{A^m}{3}$$

$$\iint_{R_m} \left[A\right] d\xi\, d\eta = \left[1, 1, 1\right] \frac{A^m}{3} \tag{D-21}$$

7. $$\iint_{R_m} \left[A\right] A_{(q)}\, d\xi\, d\eta = \iint_{R_m} \left[A_{(i)}, A_{(j)}, A_{(k)}\right] A_{(q)}\, d\xi\, d\eta$$

$$= \left[\iint_{R_m} A_{(i)} A_{(q)}\, d\xi\, d\eta,\ \iint_{R_m} A_{(i)} A_{(q)}\, d\xi\, d\eta,\ \iint_{R_m} A_{(k)} A_{(q)}\, d\xi\, d\eta\right]$$

$$\iint_{R_m} A_{(n)} A_{(q)}\, d\xi\, d\eta = \frac{1}{4A^{2m}} \iint_{R_m} \Big\{ \left[a_{1n} + a_{2n}(\xi + \bar{x}) + a_{3n}(\eta + \bar{y}) \right]$$

$$\left[a_{1q} + a_{2q}(\xi + \bar{x}) + a_{3q}(\eta + \bar{y}) \right] \Big\}\, d\xi\, d\eta$$

$$= \frac{1}{4A^{2m}} \iint_{R_m} \Big[a_{1n} a_{1q} + (a_{2n} a_{1q} + a_{1n} a_{2q})(\xi + \bar{x})$$

$$+ (a_{3n} a_{1q} + a_{1n} a_{3q})(\eta + \bar{y})$$

$$+ (a_{3n} a_{2q} + a_{2n} a_{3q})(\xi + \bar{x})(\eta + \bar{y})$$

$$+ a_{2n} a_{2q} (\xi + \bar{x})^2 + a_{3n} a_{3q} (\eta + \bar{y})^2 \Big]\, d\xi\, d\eta$$

Using the previous integration formulas we get

$$\iint_{R_m} A_{(n)} A_{(q)}\, d\xi\, d\eta = \frac{1}{4A^{2m}} \Big\{ a_{1n} a_{1q} A^m + (a_{2n} a_{1q} + a_{1n} a_{2q})\, \bar{x}\, A^m$$

$$+ (a_{3n} a_{1q} + a_{1n} a_{3q})\, \bar{y}\, A^m$$

$$+ (a_{3n} a_{2q} + a_{2n} a_{3q}) \left[\bar{x}\bar{y}\, A^m + \frac{A^m}{12} (\xi_i \eta_i + \xi_j \eta_j + \xi_k \eta_k) \right]$$

$$+ a_{2n} a_{2q} \left[\bar{x}^2 A^m + \frac{A^m}{12} (\xi_i^2 + \xi_j^2 + \xi_k^2) \right]$$

$$+ a_{3n} a_{3q} \left[\bar{y}^2 A^m + \frac{A^m}{12} (\eta_i^2 + \eta_j^2 + \eta_k^2) \right] \Big\}$$

$$= \frac{1}{4A^m} \Big\{ a_{1n} a_{1q} + (a_{2n}\, a_{1q} + a_{1n}\, a_{2q})\, \overline{x}$$

$$+ (a_{3n}\, a_{1q} + a_{1n}\, a_{3q})\, \overline{y}$$

$$+ (a_{3n}\, a_{2q} + a_{2n}\, a_{3q}) \Big[\overline{x}\,\overline{y} + \frac{1}{12} (\xi_i \eta_i + \xi_j \eta_j + \xi_k \eta_k) \Big]$$

$$+ a_{2n}\, a_{2q} \Big[\overline{x}^2 + \frac{1}{12} (\xi_i^2 + \xi_j^2 + \xi_k^2) \Big]$$

$$+ a_{3n}\, a_{3q} \Big[\overline{y}^2 + \frac{1}{12} (\eta_i^2 + \eta_j^2 + \eta_k^2) \Big] \Big\}$$

Therefore, let $\iint_{R_m} [A]\, A_{(q)}\, d\xi\, d\eta = \frac{[(AA)_q]}{4A^m}$ (D-22)

where

$$[(AA)_q] = 4A^m \Big[\iint_{R_m} A_{(i)} A_{(q)}\, d\xi\, d\eta,\ \iint_{R_m} A_{(j)} A_{(q)}\, d\xi\, d\eta,\ \iint_{R_m} A_{(k)} A_{(q)}\, d\xi\, d\eta \Big]$$

$(q = i, j, k)$

and $\iint_{R_m} A_{(n)}\, A_{(q)}\, d\xi\, d\eta$ is as given above.

<u>Derivation of matrices $[s]$ and $[p]$</u>: Combining Eq. D-15 and two other similar differentials, the expressions for the matrices $[s]$ and $[p]$ of Eq. 3-22 can be written as:

$$
[s] = \frac{D_{xx}}{4A^m}\begin{bmatrix} (a_{2i}\ a_{2i}) & (a_{2i}\ a_{2j}) & (a_{2i}\ a_{2k}) \\ (a_{2j}\ a_{2i}) & (a_{2j}\ a_{2j}) & (a_{2j}\ a_{2k}) \\ (a_{2k}\ a_{2i}) & (a_{2k}\ a_{2j}) & (a_{2k}\ a_{2k}) \end{bmatrix}
$$

$$
+ \frac{D_{xy}}{4A^m}\begin{bmatrix} (a_{3i}\ a_{2i}) & (a_{3i}\ a_{2j}) & (a_{3i}\ a_{2k}) \\ (a_{3j}\ a_{2i}) & (a_{3j}\ a_{2j}) & (a_{3j}\ a_{2k}) \\ (a_{3k}\ a_{2i}) & (a_{3k}\ a_{2j}) & (a_{3k}\ a_{2k}) \end{bmatrix}
$$

$$
+ \frac{D_{xy}}{4A^m}\begin{bmatrix} (a_{2i}\ a_{3i}) & (a_{2i}\ a_{3j}) & (a_{2i}\ a_{3k}) \\ (a_{2j}\ a_{3i}) & (a_{2j}\ a_{3j}) & (a_{2j}\ a_{3k}) \\ (a_{2k}\ a_{3i}) & (a_{2k}\ a_{3j}) & (a_{2k}\ a_{3k}) \end{bmatrix}
$$

$$
+ \frac{D_{yy}}{4A^m}\begin{bmatrix} (a_{3i}\ a_{3i}) & (a_{3i}\ a_{3j}) & (a_{3i}\ a_{3k}) \\ (a_{3j}\ a_{3i}) & (a_{3j}\ a_{3j}) & (a_{3j}\ a_{3k}) \\ (a_{3k}\ a_{3i}) & (a_{3k}\ a_{3j}) & (a_{3k}\ a_{3k}) \end{bmatrix}
$$

$$
+ \frac{u}{12}\begin{bmatrix} (a_{2i}+a_{2i}) & (a_{2i}+a_{2j}) & (a_{2i}+a_{2k}) \\ (a_{2j}+a_{2i}) & (a_{2j}+a_{2j}) & (a_{2j}+a_{2k}) \\ (a_{2k}+a_{2i}) & (a_{2k}+a_{2j}) & (a_{2k}+a_{2k}) \end{bmatrix}
$$

$$+ \frac{v}{12} \begin{bmatrix} (a_{3i} + a_{3i}) & (a_{3i} + a_{3j}) & (a_{3i} + a_{3k}) \\ (a_{3j} + a_{3i}) & (a_{3j} + a_{3j}) & (a_{3j} + a_{3k}) \\ (a_{3k} + a_{3i}) & (a_{3k} + a_{3j}) & (a_{3k} + a_{3k}) \end{bmatrix}$$

$$+ \left(\frac{u^2 + v^2}{4(D_L + D_d T)} \right) \begin{bmatrix} p \end{bmatrix} \tag{D-23}$$

where
$$\begin{bmatrix} p \end{bmatrix} = \frac{1}{4A^m} \begin{bmatrix} (AA)_i \\ (AA)_j \\ (AA)_k \end{bmatrix} . \tag{D-24}$$

APPENDIX E

PROOF OF INDEPENDENCE OF THE SYSTEM WITH RESPECT TO THE COORDINATES

The set of equations represented by Eq. 3-22 are to be applied to each triangular finite element separately. The derivations of the two square, symmetric matrices $[s]$ and $[p]$ of Eq. 3-22 are given in Appendix D.

The $[p]$ matrix for any element in Eq. 3-22 is only a function of the space coordinates of the nodal points i, j and k. The elements of the $[p]$ matrix are computed using a_1, a_2 and a_3 coefficients given by Eq. D-5 in Appendix D and space coordinates. Except a_1 coefficients, all other quantities are independent of the coordinate system because they are taken as differences of the coordinates of the nodes.

To check whether those a_1 coefficients are independent of the coordinate axis the x and y axis may be shifted by constant values, say a and b.

$$\begin{aligned} \text{Let } x_{new} &= \overline{x} = x + a \\ \text{and } y_{new} &= \overline{y} = y + b \end{aligned} \qquad \text{(E-1)}$$

where a and b are arbitrary constants. Using the relationships given by Eq. D-5 in Appendix D,

$$\text{New } a_{1i} = \bar{a}_{1i} = \bar{x}_j \bar{y}_k - \bar{x}_k \bar{y}_j$$

$$= (x_j+a)(y_k+b) - (x_k+a)(y_j+b)$$

$$= (x_j y_k - x_k y_j) + a(y_k - y_j) + b(x_j - x_k)$$

$$= a_{1i} - a\, a_{2i} - b\, a_{3i} \qquad \text{(E-2)}$$

This transformation is substituted in the expression for computing the elements of the $\left[p\right]$ matrix (Eq. D-22) and the elements are found to be invariant. The $\left[p\right]$ matrix does not change under a coordinate transformation, and hence independent of the coordinate axis.

The $\left[s\right]$ matrix is also given in Appendix D. This $\left[s\right]$ matrix is a function of $\left[p\right]$ matrix, a_2 and a_3 coefficients given by Eq. D-5, dispersion coefficients and velocity components. These a_2 and a_3 coefficients, dispersion coefficients and velocity components are independent of the coordinate transformations. The $\left[p\right]$ matrix was already proven to be independent of the coordinate system.

Thus, the whole system which results from applying Eq. 3-22 to each finite element is independent of the coordinate transformation.

APPENDIX F

NUMERICAL INTEGRATION FORMULAS

The fourth order Runge-Kutta and the Adams-Moulton multistep predictor-corrector formulas used in the numerical simulator, Eq. 3-25, are given below (Conte, 1965):

The time derivatives $\left\{\frac{\partial \phi}{\partial t}\right\}$ from Eq. 4-2 can be written as

$$\dot{\underset{\sim}{\phi}} = \underset{\sim}{f}(t, \underset{\sim}{\phi}) \tag{F-1}$$

where $\dot{\underset{\sim}{\phi}}$, $\underset{\sim}{f}$ and $\underset{\sim}{\phi}$ are vectors. The fourth order Runge-Kutta formulas are

$$\underset{\sim}{\phi}_{n+1} = \underset{\sim}{\phi}_n + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{F-2}$$

where $\underset{\sim}{k}_1 = \underset{\sim}{f}(t_n, \underset{\sim}{\phi}_n)$

$$\underset{\sim}{k}_2 = \underset{\sim}{f}\left(t_n + \frac{\Delta t}{2}, \underset{\sim}{\phi}_n + \frac{\Delta t}{2}\underset{\sim}{k}_1\right) \tag{F-3}$$

$$\underset{\sim}{k}_3 = \underset{\sim}{f}\left(t_n + \frac{\Delta t}{2}, \underset{\sim}{\phi}_n + \frac{\Delta t}{2}\underset{\sim}{k}_2\right)$$

and $\underset{\sim}{k}_4 = \underset{\sim}{f}(t_n + \Delta t, \underset{\sim}{\phi}_n + \Delta t\, \underset{\sim}{k}_3)$

where Δt is the time step size. From the initial values of $\underset{\sim}{\phi}$, four starting derivatives are computed. For subsequent time steps, the Adams-Moulton predictor formula:

$$\{\phi\}^{(0)}_{n+1} = \{\phi\}_n + \frac{\Delta t}{24}\left(55\{\frac{\partial\phi}{\partial t}\}_n - 59\{\frac{\partial\phi}{\partial t}\}_{n-1} + 37\{\frac{\partial\phi}{\partial t}\}_{n-2} - 9\{\frac{\partial\phi}{\partial t}\}_{n-3}\right)$$

(F-4)

is used and the derivatives at time level (n+1) are computed. Then using these derivatives in the Adams-Moulton corrector formula, the final corrected values of $\{\phi\}_{n+1}$ are obtained as

$$\{\phi\}^{(1)}_{n+1} = \{\phi\}_n + \frac{\Delta t}{24}\left(9\{\frac{\partial\phi}{\partial t}\}^{(0)}_{n+1} + 19\{\frac{\partial\phi}{\partial t}\}_n - 5\{\frac{\partial\phi}{\partial t}\}_{n-1} + \{\frac{\partial\phi}{\partial t}\}_{n-2}\right).$$

(F-5)

APPENDIX G

COMPUTER PROGRAM

Description of The Program

The computer program consists of five segments and the function of each segment is described below:

1. In segment one, input and data checking operations are done.
2. In segment two, the initial and boundary conditions are read and transformed using the transformation, Eq. 3-12,

   $$\phi = C \exp(\beta/2)$$

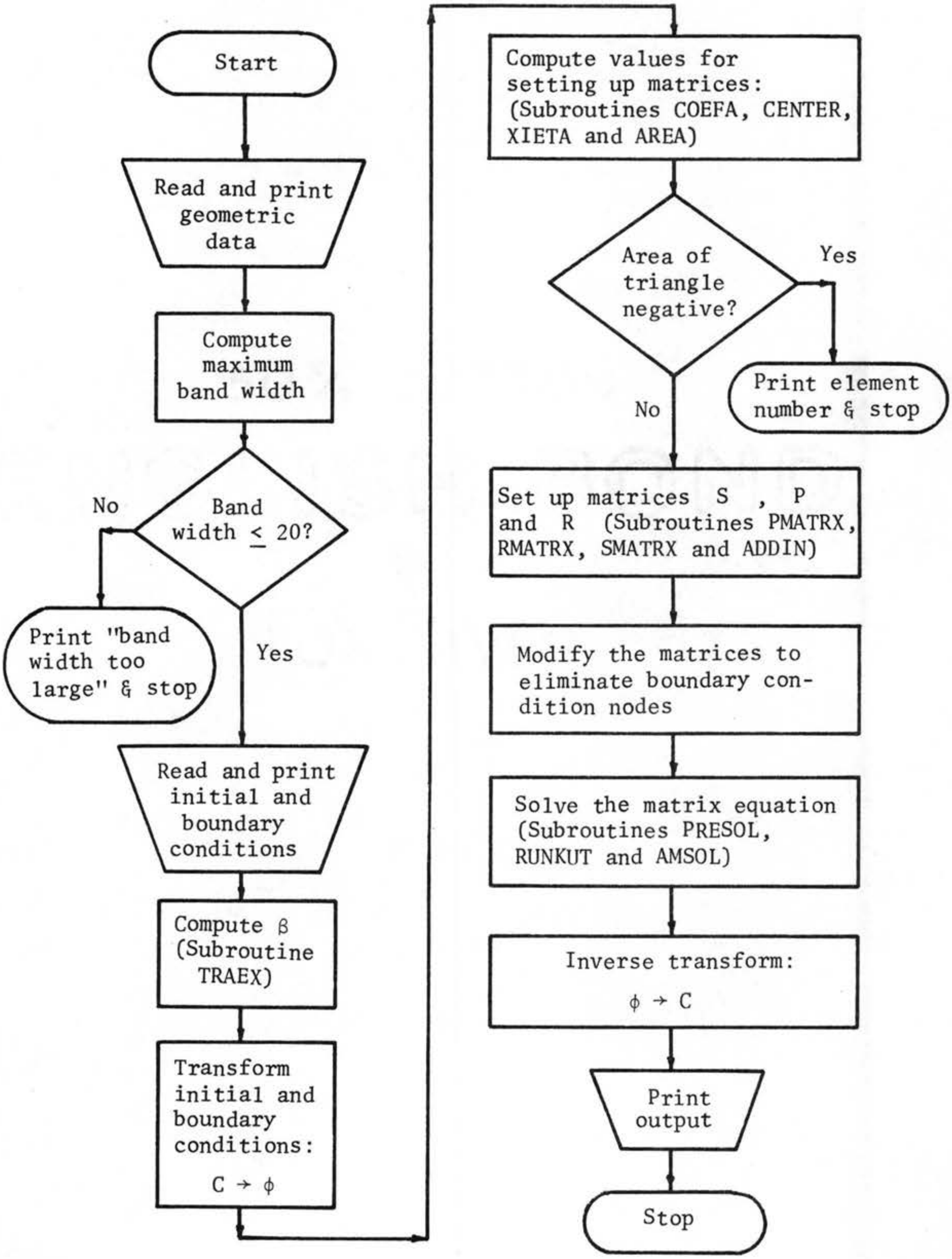
   where β is computed for any node using the medium and flow properties of the contributing elements.
3. In segment three, the matrices $[S^*]$, $[P^*]$ and $\{Q^*\}$ are formed and the matrices are modified for constant concentration (geometric) boundary conditions.
4. In segment four, the time domain solution of the system of first order linear differential equations are obtained. Numerical integration is performed utilising Runge-Kutta fourth order method and the Adams-Moulton multistep predictor-corrector method.

5. In segment five, the computed values are transformed by the inverse transformation

$$C = \phi \exp(-\beta/2)$$

and these concentration values are printed.

FLOW CHART OF THE PROGRAM



DATA INPUT FOR THE PROGRAM

1. Five title cards (16A5)

   Any information identifying the problem or blank cards.

2. First control card (3I5)

   Col. 1- 5 Number of nodes - NNOD

   Col. 6-10 Number of elements - NE

   Col. 11-15 Number of geometric boundary condition nodes - LBC

3. Second control card (4F10.0, I5)

   Col. 1-10 Starting time step for numerical integration - T

   Col. 11-20 Time segment length - TSEG

   Col. 21-30 Lower truncation error limit for numerical integration - ERRLO

   Col. 31-40 Upper truncation error limit for numerical integration - ERRHI

   Col. 41-45 Number of time segments which is equal to total time period divided by time segment length - ITT

4. Third control card (3I5)

   Col. 1- 5 1 for constant values of u and v and boundary conditions for each time segment; any other number for nonconstant values - KODE1

   Col. 6-10 1 for constant u and v over space; any other number for nonconstant values - KODE2

   Col. 11-15 1 for constant initial conditions over space; any other number for nonconstant values - KODE3

5. Element cards (5X, 3I5)

Cards must be arranged in element number sequence and all cards must have three node numbers. There should be one card for each element and node numbers must be punched from left to right in counterclockwise direction around the element.

Col. 1- 5 Element number or may be blank.

Col. 6-10 First node number of element - i

Col. 11-15 Second node number of element - j

Col. 16-20 Third node number of element - k

6. Node cards (5X, 2F10.0)

These cards contain the x and y coordinates of each node arranged in node number sequence.

Col. 1- 5 Node number or may be blank.

Col. 6-15 x coordinate of node.

Col. 16-25 y coordinate of node.

7. Initial conditions (5X, F10.0)

Cards must be arranged in node number sequence for all nodes if the columns 11-15 of third control card contains other than 1. Otherwise only one card required.

Col. 1- 5 Node number or may be blank

Col. 6-15 Initial conditions.

8. Dispersion and diffusion coefficients (4F10.0)

   This card contains the values of the longitudinal and lateral dispersion coefficients, molecular diffusion coefficient and tortuosity.

   Col. 1-10 Longitudinal dispersion coefficient - D_L

   Col. 11-20 Lateral dispersion coefficient - D_T

   Col. 21-30 Molecular diffusion coefficient - D_d

   Col. 31-40 Tortuosity - T

9. Velocity distribution (5X, 2F10.0)

   These cards must be arranged in element number sequence for all elements if columns 6-10 of third control card contains other than 1. Otherwise only one card required.

   Col. 1- 5 Element number or may be blank.

   Col. 6-15 Component of velocity in x-direction - u

   Col. 16-25 Component of velocity in y-direction - v

10. Boundary conditions (I5, F10.0)

    These cards must be arranged in sequence for the number of geometric boundary condition nodes (LBC) indicated in the first control card.

    Col. 1- 5 Node number - NBC

    Col. 6-15 Geometric boundary condition - BC

11. Repeat 9 and 10 for each time segment if columns 1-5 of third control card contains other than 1.

12. Repeat steps 1 through 11 for each additional problem.

FORTRAN IV COMPUTER PROGRAM

MAIN PROGRAM

```
      PROGRAM FINITEL
     1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C
C     ****************************************************************
C     *                                                              *
C     *   THIS PROGRAM SOLVES A TWO-DIMENSIONAL HYDRODYNAMIC         *
C     *   DISPERSION EQUATION WITH MIXED PARTIAL DERIVATIVES         *
C     *   BY FINITE ELEMENT METHOD.   TRIANGULAR ELEMENTS            *
C     *   ARE USED.  DISPERSION COEFFICIENTS ARE TREATED AS          *
C     *   SECOND ORDER SYMMETRIC TENSOR.  LONGITUDINAL AND           *
C     *   LATERAL DISPERSION COEFFICIENTS ARE INCLUDED.              *
C     *   PROVISION IS MADE TO INCLUDE MOLECULAR DIFFUSION           *
C     *   COEFFICIENT.                                               *
C     *                                                              *
C     ****************************************************************
C
C     *   FORMAT STATEMENTS
C
 1001 FORMAT (16A5/16A5/16A5/16A5/16A5)
 1002 FORMAT (3I5/4F10.0,I5/3I5)
 1003 FORMAT (5X,3I5)
 1004 FORMAT (5X,2F10.0)
 1007 FORMAT (1H1)
 1008 FORMAT (10X,15HNUMBER OF NODES,I5/10X,
     129HNUMBER OF TRIANGULAR ELEMENTS,I5/10X,
     232HSTARTING TIME SOLUTION INCREMENT,  E20.5/10X,
     323HLENGTH OF TIME SEGMENTS,  E20.5/10X,
     423HNUMBER OF TIME SEGMENTS,I5/10X,
     545HUPPER AND LOWER ERROR BOUNDS ON TIME SOLUTION,
     6  2E10.2//)
 1013 FORMAT (10X,27HDATA ERROR - ERRLO GE ERRHI//)
 1014 FORMAT (10X,43HERROR - TOO MANY NODES OR TOO MANY ELEMENTS)
 1015 FORMAT (9X,35H LIST - X AND Y COOR. FOR EACH NODE/)
 1016 FORMAT (10X,I10,  2E20.5)
 1017 FORMAT (17X,4HNODE,8X,12HX COORDINATE,8X,12HY COORDINATE/)
 1301 FORMAT (1H0,9X,21H LIST - ELEMENT NODES//)
 1302 FORMAT (10X,I10,3I5)
 1303 FORMAT (17X,3HELE,7X,5HNODES/)
 1401 FORMAT (1H0,10X,13HBAND WIDTH IS,I5//)
 1402 FORMAT (10X,33HDATA ERROR - BAND WIDTH TOO LARGE//)
 2001 FORMAT (5X,F10.0)
 2071 FORMAT (10X,37HLIST INITIAL CONDITIONS FOR EACH NODE/)
 2072 FORMAT (10X,I10,  F20.5)
 2073 FORMAT (17X,4HNODE,6X,9HINI. CON./)
 2360 FORMAT (4F10.0)
 2401 FORMAT (5X,2F10.0)
 2520 FORMAT (10X,36HLONGITUDINAL DISPERSION COEFFICIENT ,
     14HDL =,F10.5/
     210X,35HLATERAL DISPERSION COEFFICIENT DT =,F10.5/
     310X,36HMOLECULAR DIFFUSION COEFFICIENT DD =,F10.5/
     410X,17HTORTUOSITY TORT =,F10.5//)
 2601 FORMAT (9X,25H LIST VARIABLE INPUT DATA//)
 2602 FORMAT (10X,I10,  2E11.2)
 2603 FORMAT (I5,F10.0)
 2604 FORMAT (1H0,9X,25H LIST BOUNDARY CONDITIONS/)
 2605 FORMAT (15X,I5,  F20.5)
 2606 FORMAT (13X,7HELEMENT,7X,2HVX,9X,2HVY)
 2611 FORMAT (17X,4HNODE,8X,11HBOUN. COND./)
 3151 FORMAT (10X,22HNEGATIVE AREA, ELEMENT,I5)
 4001 FORMAT (9X,18H TIME SEGMENT NO. ,I5/9X,17H POSITION IN K IS,
     1I6/9X,17H TIME STEP SIZE =,  F18.8//)
 4002 FORMAT (1H1,8X,27H LIST RESULTS FOR EACH NODE//)
 5001 FORMAT (10X,4HNODE,7X,13HCONCENTRATION/)
 5201 FORMAT (9X,I5,  E20.5)
 5301 FORMAT (9X,30H------------------------------//)
C
C     *   ARRAYS
C
      DOUBLE PRECISION UT
      COMMON /BLK1/B(250,4)
      COMMON /BLK2/UT(250)
      COMMON /BLK3/S(250,20)
      COMMON /BLK4/P(250,20)
      COMMON /BLK5/R(250)
      COMMON /BLK6/NOD(250,3),X(250),Y(250)
      COMMON /BLK8/DXX(250),DYY(250),DXY(250),VX(250),VY(250)
      COMMON /BLK9/DL,DT,DD,TORT
      DIMENSION NAME(80),XLOC(3),YLOC(3),ACOF(3,3),
     1PEL(3,3),SEL(3,3),REL(3),NBC(100),BC(100),
     2U(250),BETA(250)
C
C     ****************************************************************
C     *                                                              *
C     *   SEGMENT 1                                                  *
C     *   INPUT AND DATA CHECKING                                    *
C     *                                                              *
C     ****************************************************************
C
C     *   READ TITLES, CONTROLS, AND GEOMETRIC DATA
C     *   WRITE TITLES AND CONTROL
C
 1000 READ (5,1001) (NAME(J),J=1,80)
      WRITE (6,1007)
      READ (5,1002) NNOD,NE,LBC,T,TSEG,ERRLO,ERRHI,
     1ITT,KODE1,KODE2,KODE3
      IF(NNOD.LT.250.AND.NE.LT.250.AND.LBC.LT.100) GO TO 1090
      WRITE(6,1014)
      GO TO 5500
 1090 READ (5,1003) ((NOD(I,J),J=1,3),I=1,NE)
      READ (5,1004) (X(J),Y(J),J=1,NNOD)
      WRITE (6,1001) (NAME(J),J=1,80)
      WRITE (6,1008) NNOD,NE,T,TSEG,ITT,ERRLO,ERRHI
      WRITE (6,1015)
```

```
      WRITE (6,1017)
      WRITE (6,1016) (J,X(J),Y(J),J=1,NNOD)
      IF(ERRLO.LT.ERRHI) GO TO 1300
      WRITE (6,1013)
      GO TO 5500
C
C    *   COMPUTE BAND WIDTH (NCOL)
C
 1300 NCOL=1
      WRITE (6,1301)
      WRITE (6,1303)
      DO 1400 N=1,NE
      WRITE (6,1302) N,(NOD(N,NI),NI=1,3)
      DO 1400 I=1,3
      DO 1400 J=1,3
      NN=NOD(N,I)-NOD(N,J)+1
 1400 IF(NCOL-NN.LT.0) NCOL=NN
      WRITE (6,1401) NCOL
      IF(NCOL.LE.20) GO TO 2000
      WRITE (6,1402)
      GO TO 5500
C
C    ***********************************************************
C    *                                                         *
C    *   SEGMENT 2                                             *
C    *   READ AND TRANSFORM INITIAL CONDITIONS.                *
C    *   START K LOOP WHICH SPANS REMAINDER OF PROGRAM.        *
C    *   READ VARIABLE ELEMENT DATA FOR K-TH TIME SEGMENT.     *
C    *   COMPUTE DISPERSION COEFFICIENTS FOR EACH ELEMENT.     *
C    *                                                         *
C    ***********************************************************
C
 2000 IF(KODE3.EQ.1) GO TO 2050
      READ (5,2001) (U(J),J=1,NNOD)
      GO TO 2070
 2050 READ (5,2001) U(1)
      DO 2060 J=1,NNOD
 2060 U(J)=U(1)
 2070 WRITE (6,2071)
      WRITE (6,2073)
      WRITE (6,2072) (J,U(J),J=1,NNOD)
      WRITE (6,1007)
      K=0
      NROW=NNOD
 2350 K=K+1
      TIMLTH=TSEG
      IF(KODE1.EQ.1.AND.K.GT.1) GO TO 4000
      READ (5,2360) DL,DT,DD,TORT
      IF(KODE2.EQ.1) GO TO 2440
      READ (5,2401) (VX(J),VY(J),J=1,NE)
      GO TO 2500
 2440 READ (5,2401) VX(1),VY(1)
      DO 2450 J=1,NE
      VX(J)=VX(1)
 2450 VY(J)=VY(1)
 2500 CONTINUE
      DO 2600 N=1,NE
      VEL=SQRT((VX(N)*VX(N))+(VY(N)*VY(N)))
      DXX(N)=(DL*VX(N)*VX(N)/VEL**2)+(DT*VY(N)*VY(N)/VEL**2)
     1+DD*TORT
      DYY(N)=(DT*VX(N)*VX(N)/VEL**2)+(DL*VY(N)*VY(N)/VEL**2)
     1+DD*TORT
      DXY(N)=(DL-DT)*VX(N)*VY(N)/VEL**2
 2600 CONTINUE
      WRITE (6,2601)
      WRITE (6,2520)DL,DT,DD,TORT
      WRITE (6,2606)
      WRITE (6,2602) (J,VX(J),VY(J),J=1,NE)
      CALL TRAEX(NNOD,NE, BETA)
      DO 2650 N=1,NNOD
 2650 U(N)=U(N)*EXP(BETA(N)/2.)
C
C    *   READ BOUNDARY CONDITIONS AND TRANSFORM
C
      READ (5,2603) (NBC(J),BC(J),J=1,LBC)
      WRITE (6,2604)
      WRITE (6,2611)
      WRITE (6,2605) (NBC(J),BC(J),J=1,LBC)
      DO 2900 N=1,LBC
      I=NBC(N)
 2900 BC(N)=BC(N)*EXP(BETA(I)/2.)
C
C    ***********************************************************
C    *                                                         *
C    *   SEGMENT 3                                             *
C    *   BUILD SYSTEM MATRICES  S, P, AND R AND SET            *
C    *   BOUNDARY CONDITIONS IN MATRICES.                      *
C    *                                                         *
C    ***********************************************************
C
      M = 0
      DO 3000 I = 1,NROW
      R(I)=0.
      DO 3000 J = 1,NCOL
      S  (I,J) = 0.0
 3000 P  (I,J) = 0.0
 3100 M = M+1
      CALL COEFA (M,ACOF)
      CALL CENTER (M, XBAR, YBAR)
      CALL XIETA(M,XBAR,YBAR,XLOC,YLOC)
      CALL AREA(XLOC,YLOC,AM)
      IF(AM.GT.0.) GO TO 3150
      WRITE (6,3151) M
      GO TO 5500
 3150 CALL PMATRX(AM,ACOF,XBAR,YBAR,XLOC,YLOC,PEL)
      CALL RMATRX(M,PEL)
      CONSS=(((VX(M)**2+VY(M)**2)/(DL+DD*TORT))/4.0)
      CALL SMATRX(M,AM,CONSS,PEL,SEL,ACOF)
      CALL ADDIN (SEL,PEL,REL,M)
      IF (M .LT.NE) GO TO 3100
```

```
C
C     *   SET BOUNDARY CONDITIONS IN MATRICES
C
      DO 3230 I = 1,LBC
      NN = NBC(I)
      NC = NCOL
 3200 NR = NN-NC+1
      IF (NR .LT. 1) GO TO 3210
      P (NR) = P (NR) - S  (NR,NC)*BC   (I)
 3210 NC = NC-1
      IF (NC .GT. 1) GO TO 3200
      NC = 1
      NR = NN
 3220 NR = NR+1
      IF (NR .GT. NROW) GO TO 3230
      NC = NC+1
      IF (NC .GT. NCOL) GO TO 3230
      P (NR) = P (NR)-S  (NN,NC)*BC   (I)
      GO TO 3220
 3230 CONTINUE
C
C     *   REFORM MATRICES AND ELIMINATE EQUATIONS
C     *   AT BOUNDARY CONDITION NODES
C
      DO 3300 I = 1,LBC
      NN = NBC(I)-I+1
      NROW = NROW-1
      IF (NN .GE. NROW) GO TO 3300
      DO 3240 NR = NN,NROW
        U(NR) =     U(NR+1)
        P(NR) =     P(NR+1)
      DO 3240 NC = 1,NCOL
       S (NR,NC) =  S (NR+1,NC)
 3240  P (NR,NC) =  P (NR+1,NC)
 3250 NR = NN
      N = 2
 3260 NR = NR-1
      IF (NR .LT. 1) GO TO 3300
      N = N+1
      IF (N .GT. NCOL ) GO TO 3280
      DO 3270 J = N,NCOL
        P(NR, J-1) =   P(NR,J)
 3270   S(NR, J-1) =   S(NR,J)
        P(NR,NCOL) = 0.0
        S(NR,NCOL) = 0.0
      GO TO 3260
 3280   S(NR,NCOL) = 0.0
        P(NR,NCOL) = 0.0
 3300 CONTINUE
```

```
C
C     ****************************************************************
C     *                                                              *
C     *   SEGMENT 4                                                  *
C     *   TIME DOMAIN SOLUTION OF SYSTEM OF FIRST ORDER.             *
C     *   LINEAR ORDINARY DIFFERENTIAL EQUATIONS WITH                *
C     *   CONSTANT COEFFICIENTS.  SUBROUTINES RUNKUT AND             *
C     *   AMSOL ARE USED FOR NUMERICAL INTEGRATION SCHEME            *
C     *   FOR THE K-TH TIME SEGMENT.  TIME STEP AUTOMATICALLY        *
C     *   ADJUSTED FOR OPTIMUM CONVERGENCE.                          *
C     *                                                              *
C     ****************************************************************
C
      CALL PRESOL (NROW, NCOL)
 4000 LL = 0
      WRITE (6,4002)
C
C     *   COMPUTE NUMBER OF TIME STEPS IN K-TH TIME SEGMENT
C     *   AND ADJUST TIME SIZE AS REQUIRED.
C
 4100 NSTEP=TIMLTH/T+0.5
      STEP=NSTEP
      T=TIMLTH/STEP
      WRITE (6,4001) K,LL,T
      IF (NSTEP .GE. 4) GO TO 4200
      T=T/2.
      GO TO 4100
C
C     *   COMPUTE STARTING VALUES FOR AMSOL
C
 4200 CALL RUNKUT (U    , NROW, NCOL, T)
      LL = 3
C
C     *   AMSOL CALCS ALL OTHER VALUES OF FUNCTION IN K-TH
C     *   TIME SEGMENT AND CHECKS MAX. TRUNCATION ERROR IN
C     *   SYSTEM FOR AUTOMATIC ADJUSTMENT OF TIME STEP SIZE.
C
 4300 LL = LL + 1
      CALL AMSOL (NROW, NCOL, T,TRUNK,U)
      IF (LL .LT. 6) GO TO 4400
      IF (TRUNK .GE. ERRLO    .AND. TRUNK .LE. ERRHI) GO TO 4400
      IF (TRUNK .LT. ERRLO  ) GO TO 4320
      LL=LL-1
      DIFTIM=NSTEP-LL
      TIMLTH=DIFTIM*T
      T=T/2.
      GO TO 4100
 4320 DIFTIM=NSTEP-LL
      IF (DIFTIM .LT. 16.00005) GO TO 4400
      TIMLTH=DIFTIM*T
      T=T*2.
      DO 4330 I=1,NROW
 4330    U(I)=UT(I)
      GO TO 4100
 4400 IF(LL .LT. NSTEP) GO TO 4300
```

```
C
C     ****************************************************************
C     *                                                              *
C     *   SEGMENT 5                                                  *
C     *   TRANSFORMS AND OUTPUTS RESULTS                             *
C     *                                                              *
C     ****************************************************************
C
 5000 WRITE (6,5001)
      N=0
      J=0
      DO 5050 I=1,LBC
      II=NBC(I)
 5050 U(II)=BC(I)*EXP(-BETA(II)/2.)
 5100 N=N+1
      J=J+1
      DO 5200 I=1,LBC
      IF (NBC(I).EQ.J) J=J+1
 5200 CONTINUE
      IF (J.GT.NNOD) GO TO 5300
         U(J)=UT(N)
      U(J) =U(J)*EXP(-BETA(J)/2.)
      WRITE (6,5201) J,U(J)
      IF (N.LT.NROW) GO TO 5100
 5300 WRITE (6,5301)
      IF(KODE1.EQ.1) GO TO 5350
      GO TO 5400
 5350 DO 5360 J=1,NROW
 5360 U(J)=UT(J)
 5400 IF(K.LT.ITT) GO TO 2350
      GO TO 1000
 5500 STOP
      END
```

SUBROUTINE XIETA

```
      SUBROUTINE XIETA(M,XBAR,YBAR,XLOC,YLOC)
C
C     ****************************************************************
C     *                                                              *
C     *   THIS SUBROUTINE COMPUTES THE LOCAL COORDINATES             *
C     *   OF NODES ON TRIANGULAR ELEMENT M.                          *
C     *                                                              *
C     ****************************************************************
C
      COMMON /BLK6/NOD(250,3),X(250),Y(250)
      DIMENSION XLOC(3),YLOC(3)
      DO 100 L=1,3
      I=NOD(M,L)
      XLOC(L)=X(I)-XBAR
  100 YLOC(L)=Y(I)-YBAR
      RETURN
      END
```

SUBROUTINE COEFA

```
      SUBROUTINE COEFA(M,ACOF)
C
C     ****************************************************************
C     *                                                              *
C     *   THIS SUBROUTINE COMPUTES THE A-COEFFICIENTS                *
C     *   FOR THE MATRICES OF THE M-TH ELEMENT.                      *
C     *                                                              *
C     ****************************************************************
C
      COMMON /BLK6/NOD(250,3),X(250),Y(250)
      DIMENSION ACOF(3,3)
      J1=NOD(M,1)
      J2=NOD(M,2)
      J3=NOD(M,3)
      ACOF(1,1) = X(J2)*Y(J3)-Y(J2)*X(J3)
      ACOF(1,2) = X(J3)*Y(J1)-Y(J3)*X(J1)
      ACOF(1,3) = X(J1)*Y(J2)-Y(J1)*X(J2)
      ACOF(2,1) = Y(J2)-Y(J3)
      ACOF(2,2) = Y(J3)-Y(J1)
      ACOF(2,3) = Y(J1)-Y(J2)
      ACOF(3,1) = X(J3)-X(J2)
      ACOF(3,2) = X(J1)-X(J3)
      ACOF(3,3) = X(J2)-X(J1)
      RETURN
      END
```

SUBROUTINE COMB

```
      SUBROUTINE COMB (Y, NROW, NCOL, Z)
C
C     ****************************************************************
C     *                                                              *
C     *   THIS SUBROUTINE MULTIPLIES SYMMETRIC MATRIX S              *
C     *   TO MATRIX Y AND STORES THE RESULT IN Z.                    *
C     *                                                              *
C     ****************************************************************
C
      COMMON /BLK3/S(250,20)
      DIMENSION Y(250),Z(250)
      DO 200 I=1,NROW
      Z(I)=Y(I)*  S(I,1)
      DO 200 K=2,NCOL
      L=I-K+1
      IF (L .LT. 1) GO TO 100
      Z(I)=Z(I)+Y(L)*  S(L,K)
  100 N=I+K-1
      IF (N.GT. NROW) GO TO 200
      Z(I)=Z(I)+Y(N)*  S(I,K)
  200 CONTINUE
      RETURN
      END
```

SUBROUTINE TRAEX

```
      SUBROUTINE TRAEX(NNOD,NE, BETA)
C
C     **********************************************************
C     *                                                        *
C     *   THIS SUBROUTINE COMPUTES THE BETA TRANSFORM FUNCTION *
C     *                                                        *
C     **********************************************************
C
      COMMON /BLK6/NOD(250,3),X(250),Y(250)
      COMMON /BLK8/DXX(250),DYY(250),DXY(250),VX(250),VY(250)
      COMMON /BLK9/DL,DT,DD,TORT
      DIMENSION BETA(250)
      DO 300 N=1,NNOD
      DN=0.
      VVX=0.
      VVY=0.
      DO 200 I=1,NE
      DO 200 J=1,3
      IF(NOD(I,J).EQ.N) GO TO 100
      GO TO 200
  100 DN=DN+1.
      VVX=VVX+VX(I)
      VVY=VVY+VY(I)
  200 CONTINUE
      VVX=VVX/DN
      VVY=VVY/DN
  300 BETA(N)=-(VVX*X(N)+VVY*Y(N))/(DL+DD*TORT)
      RETURN
      END
```

SUBROUTINE CENTER

```
      SUBROUTINE CENTER (M,XBAR,YBAR)
C
C     **********************************************************
C     *                                                        *
C     *   THIS SUBROUTINE COMPUTES THE CENTER COORDINATE       *
C     *   OF TRIANGULAR ELEMENT M.                             *
C     *                                                        *
C     **********************************************************
C
      COMMON /BLK6/NOD(250,3),X(250),Y(250)
      I=NOD(M,1)
      J=NOD(M,2)
      K=NOD(M,3)
      XBAR=(X(I)+X(J)+X(K))/3.
      YBAR=(Y(I)+Y(J)+Y(K))/3.
      RETURN
      END
```

SUBROUTINE AREA

```
      SUBROUTINE AREA(XLOC,YLOC,AM)
C
C     **********************************************************
C     *                                                        *
C     *   THIS SUBROUTINE CALCULATES THE AREA OF               *
C     *   TRIANGULAR ELEMENT M.                                *
C     *                                                        *
C     **********************************************************
C
      DIMENSION XLOC(3),YLOC(3)
      AM=(XLOC(2)*YLOC(3)-XLOC(3)*YLOC(2)-XLOC(1)*
     1   YLOC(3)+XLOC(3)*YLOC(1)+XLOC(1)*YLOC(2)
     2   -XLOC(2)*YLOC(1))/2.
      RETURN
      END
```

SUBROUTINE SMATRX

```
      SUBROUTINE SMATRX (M,AM,CONS5,PEL,SEL,ACOF)
C
C     **********************************************************
C     *                                                        *
C     *   THIS SUBROUTINE CONSTRUCTS THE S MATRIX FOR          *
C     *   THE M-TH TRIANGULAR ELEMENT.                         *
C     *   MATRIX IS SYMMETRICAL.                               *
C     *                                                        *
C     **********************************************************
C
      COMMON /BLK8/DXX(250),DYY(250),DXY(250),VX(250),VY(250)
      DIMENSION PEL(3,3),SEL(3,3),ACOF(3,3)
      DO 100 I=1,3
      DO 100 J=1,3
  100 SEL(I,J)=0.
      CONS1 =DXX(M)/(4.0*AM)
      CONS12=DXY(M)/(4.0*AM)
      CONS2 =DYY(M)/(4.0*AM)
      CONS3=VX(M)/12.
      CONS4=VY(M)/12.
      DO 300 L=1,3
      DO 300 N=1,3
      SEL(L,N)=SEL(L,N)+(ACOF(2,L)*ACOF(2,N))*CONS1
      SEL(L,N)=SEL(L,N)+(ACOF(3,L)*ACOF(2,N))*CONS12
      SEL(L,N)=SEL(L,N)+(ACOF(2,L)*ACOF(3,N))*CONS12
      SEL(L,N)=SEL(L,N)+(ACOF(3,L)*ACOF(3,N))*CONS2
      SEL(L,N)=SEL(L,N)+(ACOF(2,L)+ACOF(2,N))*CONS3
      SEL(L,N)=SEL(L,N)+(ACOF(3,L)+ACOF(3,N))*CONS4
  300 SEL(L,N)=SEL(L,N)+CONS5*PEL(L,N)
      RETURN
      END
```

SUBROUTINE RMATRX

```
      SUBROUTINE RMATRX(M,REL)
C
C     **************************************************************
C     *                                                            *
C     *   THIS SUBROUTINE CONSTRUCTS THE R MATRIX                  *
C     *   FOR THE M-TH ELEMENT.  WHEN THERE IS NO SINK THE         *
C     *   COEFFICIENTS OF R MATRIX ARE ZERO                        *
C     *                                                            *
C     **************************************************************
C
      DIMENSION REL(3)
      DO 100 J=1,3
  100 REL(J)=0.0
      RETURN
      END
```

SUBROUTINE ADDIN

```
      SUBROUTINE ADDIN (SEL,PEL,REL,M)
C
C     **************************************************************
C     *                                                            *
C     *   THIS SUBROUTINE CONSTRUCTS THE MAIN SYSTEM MATRICES      *
C     *   WHICH ARE SYMMETRICAL AND IN BAND FORM                   *
C     *                                                            *
C     **************************************************************
C
      COMMON /BLK3/S(250,20)
      COMMON /BLK4/P(250,20)
      COMMON /BLK5/R(250)
      COMMON /BLK6/NOD(250,3),X(250),Y(250)
      DIMENSION SEL(3,3),PEL(3,3),REL(3)
      DO 200 J=1,3
      NR=NOD(M,J)
      DO 100 K=1,3
      NC=NOD(M,K)-NOD(M,J)+1
      IF(NC.LE.0) GO TO 100
        S(NR,NC)=  S(NR,NC)+SEL(J,K)
        P(NR,NC)=  P(NR,NC)+PEL(J,K)
  100 CONTINUE
  200 R(NR)=R(NR)+REL(J)
      RETURN
      END
```

SUBROUTINE PRESOL

```
      SUBROUTINE PRESOL (NROW, NCOL)
C
C     **************************************************************
C     *                                                            *
C     *   THIS SUBROUTINE PRE-TRIANGULARIZES A SYMMETRIC           *
C     *   MATRIX IN BAND FORM FOR SOLUTION BY THE GAUSSIAN         *
C     *   ELIMINATION METHOD.  FINAL SOLUTION IS BY                *
C     *   SUBROUTINE FINSOL.                                       *
C     *                                                            *
C     **************************************************************
C
      COMMON /BLK4/P(250,20)
      DIMENSION ST(20)
      N = 0
  100 N=N+1
C
C     *   REDUCE PIVOT EQUATIONS
C
      IF (N-NROW) 150,300,150
  150 DO 200 K=2,NCOL
      ST(K)=  P(N,K)
  200   P(N,K) =    P(N,K)/  P(N,1)
C
C     *   REDUCE REMAINING EQUATIONS
C
      DO 260 L=2,NCOL
      I=N+L-1
      IF (NROW-I) 260,240,240
  240 J=0
      DO 250 K=L,NCOL
      J=J+1
  250   P(I,J)=   P(I,J)-ST(L)*  P(N,K)
  260 CONTINUE
      GO TO 100
  300 RETURN
      END
```

SUBROUTINE RUNKUT

```
      SUBROUTINE RUNKUT (U, NROW, NCOL, TSTEP)
C
C     ***************************************************************
C     *                                                             *
C     *   THIS SUBROUTINE IS A FOURTH ORDER RUNGE-KUTTA SOLUTION    *
C     *   FOR AN M-TH ORDER SYSTEM OF FIRST ORDER EQUATIONS WITH    *
C     *   CONSTANT COFF THAT ARE SYMMETRIC AND IN BAND FORM.        *
C     *   COMPUTATIONS ARE IN PARTIAL DOUBLE PRECISION              *
C     *   THE PROGRAM IS A STARTER FOR THE ADAMS-MOULTON METHOD.    *
C     *   THIS SUBROUTINE REQUIRES SUBROUTINES COMB AND FINSOL.     *
C     *   THIS PROGRAM HAS COMMON STORAGE.                          *
C     *                                                             *
C     ***************************************************************
C
      DOUBLE PRECISION DVAR, UT
      COMMON /BLK1/B(250,4)
      COMMON /BLK2/UT(250)
      COMMON /BLK3/S(250,20)
      COMMON /BLK4/P(250,20)
      COMMON /BLK5/SL(250)
      DIMENSION F(250),U(250),G(250),A(250,3)
      DO 100 I=1,NROW
  100 UT(I)=U(I)
C
C     *   COMPUTE SINGLE PRECISION DERIVATIVES
C
      DO 1000 K=1,4
      CALL COMB (U, NROW, NCOL, F)
      DO 101 I=1,NROW
  101 F(I)=SL(I)-F(I)
      CALL FINSOL (F, NROW, NCOL)
      DO 102 I=1,NROW
  102 B(I,K)=F(I)
      IF (K .GE. 4) RETURN
C
C     *   COMPUTE THREE ADDITIONAL SINGLE PRECISION
C     *   COEFFICIENTS FOR RUNKUT
C
      DO 104 I=1,NROW
  104 G(I)=U(I)+B(I,K)*TSTEP/2.0
      CALL COMB (G, NROW, NCOL, F)
      DO 105 I=1,NROW
  105 F(I)=SL(I)-F(I)
      CALL FINSOL (F, NROW, NCOL)
      DO 106 I=1,NROW
  106 A(I,1)=F(I)
      DO 107 I=1,NROW
  107 G(I)=U(I)+A(I,1)*TSTEP/2.0
      CALL COMB (G, NROW, NCOL, F)
      DO 108 I=1,NROW
  108 F(I)=SL(I)-F(I)
      CALL FINSOL (F, NROW, NCOL)
      DO 109 I=1,NROW
  109 A(I,2)=F(I)
      DO 110 I=1,NROW
  110 G(I)=U(I)+A(I,2)*TSTEP
      CALL COMB (G, NROW, NCOL, F)
      DO 111 I=1,NROW
  111 F(I)=SL(I)-F(I)
      CALL FINSOL (F, NROW, NCOL)
      DO 112 I=1,NROW
  112 A(I,3)=F(I)
C
C     *   COMPUTE VALUE OF FUNCTION IN DOUBLE PRECISION
C
      DO 1000 I=1,NROW
      DVAR=TSTEP*(B(I,K)+2.0*(A(I,1)+A(I,2))+A(I,3))/6.0
      UT(I)=UT(I)+DVAR
 1000 U(I)=UT(I)
      END
```

SUBROUTINE PMATRX

```
      SUBROUTINE PMATRX(AM,ACOF,XBAR,YBAR,XLOC,YLOC,PEL)
C
C     ***************************************************************
C     *                                                             *
C     *   THIS SUBROUTINE CONSTRUCTS A SYMMETRICAL                  *
C     *    P      MATRIX FOR THE M-TH TRIANGULAR ELEMENT.           *
C     *                                                             *
C     ***************************************************************
C
      DIMENSION ACOF(3,3),XLOC(3),YLOC(3),PEL(3,3)
      CONS1=XBAR*YBAR+(XLOC(1)*YLOC(1)+XLOC(2)*YLOC(2)
     1      +XLOC(3)*YLOC(3))/12.
      CONS2=ABS(XBAR**2+(XLOC(1)**2+XLOC(2)**2
     1      +XLOC(3)**2)/12.)
      CONS3=ABS(YBAR**2+(YLOC(1)**2+YLOC(2)**2
     1      +YLOC(3)**2)/12.)
      DO 200 L=1,3
      DO 200 N=1,3
      PEL(L,N)=(ACOF(1,N)*ACOF(1,L)+(ACOF(2,N)*ACOF(1,L)
     1          +ACOF(1,N)*ACOF(2,L))*XBAR+(ACOF(3,N)*
     2          ACOF(1,L)+ACOF(1,N)*ACOF(3,L))*YBAR+
     3          (ACOF(3,N)*ACOF(2,L)+ACOF(2,N)*ACOF(3,L))
     4          *CONS1+ACOF(2,N)*ACOF(2,L)*CONS2
     5          +ACOF(3,N)*ACOF(3,L)*CONS3)/(4.*AM)
  200 CONTINUE
      RETURN
      END
```

SUBROUTINE AMSOL

```
      SUBROUTINE AMSOL (M, NCOL, T,TRUNK,UEND)
C
C     ******************************************************
C     *                                                    *
C     *   THIS SUBROUTINE SOLVES AN N-TH ORDER SYSTEM OF   *
C     *   FIRST ORDER EQUATIONS WITH CONSTANT COEF IN      *
C     *   BAND FORM BY THE ADAMS-MOULTON PREDICTOR-CORRECTOR *
C     *   METHOD.  THIS PROGRAM REQUIRES FOUR STARTING     *
C     *   DERIVATIVES TO BEGIN COMPUTATIONS  FOR A SINGLE  *
C     *   ADDITIONAL TIME STEP.                            *
C     *   COMPUTATIONS ARE IN PARTIAL DOUBLE PRECISION     *
C     *   THIS PROGRAM REQUIRES SUBROUTINES COMB AND FINSOL. *
C     *   THIS PROGRAM HAS COMMON STORAGE REQUIREMENTS.    *
C     *                                                    *
C     ******************************************************
C
      DOUBLE PRECISION DVAR, UT
      COMMON /BLK1/B(250,4)
      COMMON /BLK2/UT(250)
      COMMON /BLK3/S(250,20)
      COMMON /BLK4/P(250,20)
      COMMON /BLK5/SL(250)
      DIMENSION U(250),F(250),UEND(250)
      TRUNK=0.0
      DO 100 I=1,M
      UEND(I)=UT(I)
  100 U(I)=UEND(I)+T*(B(I,1)*55.-B(I,2)*59.+B(I,3)*37.
     1 -B(I,4)*9.)/24.
      CALL COMB (U,     M, NCOL, F)
      DO 101 I=1,M
  101 F(I)=SL(I)-F(I)
      CALL FINSOL (F, M, NCOL)
      DO 102 I=1,M
      DVAR=T*(F(I)*9.+B(I,1)*19.-B(I,2)*5.+B(I,3))/24.
      UT(I)=UT(I)+DVAR
      USAVE=U(I)
      U(I)=UT(I)
      EXOR=ABS(USAVE-U(I))
      IF (EXOR .GT. TRUNK) TRUNK=EXOR
  102 CONTINUE
      CALL COMB (U,     M, NCOL, F)
      DO 104 I=1,M
  104 F(I)=SL(I)-F(I)
      CALL FINSOL (F, M, NCOL)
      DO 105 I=2,4
      DO 105 J=1,M
  105 B(J,I-1)=B(J,I)
      DO 106 I=1,M
  106 B(I,4)=F(I)
      TRUNK=TRUNK/14.
      RETURN
      END
```

SUBROUTINE FINSOL

```
      SUBROUTINE FINSOL ( SS, NROW, NCOL)
C
C     ******************************************************
C     *                                                    *
C     *   THIS SUBROUTINE SOLVES A SET OF LINEAR SIMULTANEOUS *
C     *   EQUATIONS WHOSE COEFFICIENT MATRIX HAS BEEN      *
C     *   PRE-TRIANGULARIZED BY THE GAUSSIAN ELIMINATION METHOD*
C     *   THE SYSTEM MATRIX IS IN BAND FORM AND IS SYMMETRICAL.*
C     *   SOLUTION IS PLACED IN THE LOAD MATRIX.           *
C     *                                                    *
C     ******************************************************
C
      COMMON /BLK4/P(250,20)
      DIMENSION SS(250)
C
C     *   REDUCE LOAD VARIABLES
C
      DO 100 N=1,NROW
      DO 100 K=2,NCOL
      L=N-K+1
      IF (L .LT. 1) GO TO 100
       SS(N)= SS(N)- SS(L)*  P(L,K)
  100 CONTINUE
      DO 200 N=1,NROW
  200  SS(N)= SS(N)/  P(N,1)
C
C     *   BACK SUBSTITUTION
C
      N=NROW
  300 N=N-1
      IF (N) 350,500,350
  350 DO 400 K=2,NCOL
      L=N+K-1
      IF (NROW-L) 400,370,370
  370  SS(N)= SS(N)-  P(N,K)* SS(L)
  400 CONTINUE
      GO TO 300
  500 RETURN
      END
```

APPENDIX H

EXAMPLES TO SHOW INSTABILITY

Results for problem in Fig. 4-8 with $D_L = 0.01\ cm^2/sec.$:

The numerical results for the problem in Fig. 4-8 with the longitudinal dispersion coefficient $D_L = 0.01\ cm^2/sec$ is given in Table H-I. A comparison of results in Table H-I and that in Figs. 4-9, 4-10 and 4-11 indicate the influence of the dispersion coefficient D_L upon the stability of the solution.

TABLE H-I

Values of C/C_o for problem shown in Fig. 4-8

$l = 10.0$ cm

$D_L = 0.01\ cm^2/sec$

$V = 0.1$ cm/sec

$t = 10.0$ secs

Fractional Distance x'/l	Numerical Solutions C/C_o
0	1.0
0.2	-7.5856×10^3
0.4	-2.8267×10^7

TABLE H-I (Cont'd)

Fractional Distance	Numerical Solutions
0.6	8.9563×10^{11}
0.8	-4.0849×10^{15}
1.0	7.8542×10^{19}
	-1.0212×10^{20}

Results for problem in Figs. 4-1 and 4-2: The problem shown in Figs. 4-1 and 4-2 was solved using the method of Guymon (1970) and a longitudinal dispersion coefficient $D_L = 0.0012$ sq. miles/year which is equivalent to $D_L = 1.0\ cm^2/sec$ instead of using $D_L = 0.5656$ sq. miles/year.

The $\left[S\right]$ and $\left[S\right]^{-1}$ matrices for this case are shown below:

$$\left[S\right] = \begin{bmatrix} 3.93 & 0 & 0.981 & 0.981 & 0 & 0 & 0 \\ 0 & 3.93 & 0 & 0.981 & 0.981 & 0 & 0 \\ 0.981 & 0 & 3.93 & 0.982 & 0 & 0.981 & 0 \\ 0.981 & 0.981 & 0.982 & 7.86 & 0.982 & 0.981 & 0.981 \\ 0 & 0.981 & 0 & 0.982 & 3.93 & 0 & 0.981 \\ 0 & 0 & 0.981 & 0.981 & 0 & 3.93 & 0 \\ 0 & 0 & 0 & 0.981 & 0.981 & 0 & 3.93 \end{bmatrix}$$

$$[S]^{-1} =$$

$$\begin{bmatrix}
0.279 & 0.00678 & -0.068 & -0.0317 & 0.00454 & 0.0249 & 0.00678 \\
0.00678 & 0.279 & 0.00454 & -0.0317 & -0.068 & 0.00678 & 0.0249 \\
-0.068 & 0.00454 & 0.294 & -0.0212 & 0.00304 & -0.068 & 0.00454 \\
-0.0317 & -0.0317 & -0.0212 & 0.148 & -0.0212 & -0.0317 & -0.0317 \\
0.00454 & -0.068 & 0.00304 & -0.0212 & 0.294 & 0.00454 & 0.068 \\
0.0249 & 0.00678 & -0.068 & -0.0317 & 0.00454 & 0.279 & 0.00678 \\
0.00678 & 0.0249 & 0.00454 & -0.0317 & -0.068 & 0.00678 & 0.279
\end{bmatrix}$$

The results are shown in Table H-II for the same values of the fractional distance for which the results are given in Table I. A comparison of results shown in Tables I and H-II indicate the influence of the dispersion coefficient D_L upon the stability.

TABLE H-II

Values of C/C_o for problem in Figs. 4-1 and 4-2 at time = 5 years. Longitudinal dispersion coefficient $D_L = 1.0\ cm^2/sec$

Fractional Distance	Numerical Solutions
x'/l	C/C_o
0	1.0
0.25	-7.848×10^{35}
0.5	-7.994×10^{68}
0.75	6.276×10^{104}
1.0	0.148

APPENDIX I

LIST OF SYMBOLS

Symbol	Definition	Units
A	Area of triangular element	L^2
$[A]$	A row matrix	--
$a_{i,j}$	Coefficients of $[S]$ matrix used in stability analysis	--
a_{bn}	Coefficient for deriving $[s]$ and $[p]$ matrices	--
C	Mass concentration of tracer	FT^2L^{-4}
C_o	Reference concentration	FT^2L^{-4}
D	Diffusion coefficient	L^2T^{-1}
D_{ij}	Dispersion coefficient	L^2T^{-1}
D^*_{ij}	Total dispersion coefficient	L^2T^{-1}
D_L	Longitudinal dispersion coefficient	L^2T^{-1}
D_s	Dispersion coefficient in the s-direction	L^2T^{-1}
D_T	Lateral dispersion coefficient	L^2T^{-1}
D_d	Molecular diffusion coefficient	L^2T^{-1}
d	Characteristics of porous medium	L
d^*	Particle size of porous medium	L
i	Indicates node; also used as a subscript	--
j	Indicates node; also used as a subscript	--
i, j	Index coordinates used to denote tensor	--

Symbol	Definition	Units
k	Indicates node	--
K	Permeability	L^2
L	Number of nodes with geometric boundary conditions	--
l	Length of column of porous medium	L
m	Indicates m^{th} finite element; used as a superscript or subscript	--
N	Total number of nodal points	--
n	Indicates n^{th} node or it may indicate normal direction	--
$[P^*]$	A square, symmetric matrix	--
$[P]$	A square, symmetric matrix	--
$[p]$	A square, symmetric submatrix of $[P^*]$ relating to one particular finite element	--
$\{Q^*\}$	A column matrix	--
$\{Q\}$	A column matrix	--
q_n^*	Elements of the column matrix $\{Q^*\}$	--
q_n	Elements of the column matrix $\{Q\}$	--
R	Two-dimensional region	L^2
R_m	Region of the m^{th} triangular finite element	L^2
r	Radius	L
$[S^*]$	A square, symmetric matrix	--
$[S]$	A square, symmetric matrix	--
$[s]$	A square, symmetric submatrix of $[S^*]$ relating to one particular finite element	--

Symbol	Definition	Units
T	Tortuosity	--
t	Time	T
u	Seepage velocity in x-direction	LT^{-1}
v	Seepage velocity in y-direction	LT^{-1}
V	Magnitude of seepage velocity vector	LT^{-1}
V_s	Magnitude of seepage velocity vector in s-direction	LT^{-1}
x, y	Cartesian space coordinates	L
x', y'	Rotated Cartesian space coordinates	L
$\alpha_1, \alpha_2, \alpha_3$	Coefficients of linear polynomial in x and y	--
β	An argument in the reducing factor $\exp(\beta)$	--
δ	Denotes a small variation	--
∂	Denotes a differential operator	--
ξ	Local x-coordinate	L
η	Local y-coordinate	L
θ	Angle through which the x and y axes are rotated	--
ϕ	Transformed C	FT^2L^{-4}
ϕ_o	Transformed C_o	FT^2L^{-4}
μ	Viscosity	FTL^{-2}
ν	Kinematic viscosity	L^2T^{-1}
Φ	Potential function	--
ψ	Stream function	--
erf	Error function	--
erfc	Complimentary error function	--

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