Dissertation

GALERKIN SIMULATION OF HYDRODYNAMIC DISPERSION

Submitted by

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In partial fulfillment of the requirements

for the Degree of Doctor of Philosophy

Colorado State University

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April, 1974

CED73-74AP17

To my parents.

ABSTRACT

The problem of predicting salt-content of waters pumped by fully or partially penetrating wells in an aquifer, contaminated by salt-water intrusion on sea-coasts, indiscriminate pumping of deep saline aquifers or waste-water recharge over prolonged periods of time, has demanded the attention of hydraulic engineers and geohydrologists for the last two decades or so. This investigation is an attempt to develop a new approach for modeling such situations.

A numerical simulator has been developed to represent the problem of salt-water movement induced by pumping from a saturated elastic aquifer. This simulator is based upon the Galerkin-finite-element formulations of the flow and convective-dispersion equations in cylindrical polar coordinates. Appropriate flow and convective-dispersion equations have been derived from first principles in tensorial form, taking the tensorial nature of dispersion and molecular diffusion into account. Finite-element-formulations have been developed for both the equations following the Galerkin-weighted-residual process both for the space and time domains. The flow equation formulation results in a system of symmetric matrices and that for the convective-dispersion equation in a system of non-symmetric matrices. Both these systems have been solved by Gauss-elimination. The flow and convective-dispersion equations are solved in sequence following the leap-frog-technique.

The numerical simulator consists of three computer programs; MESH, FLOW and DISPER. Program MESH is an automatic generation scheme for a suitable mesh layout with triangular elements, given the geometry of the flow region. This program incorporates an optimization scheme for

band-width reduction. The other two programs, FLOW and DISPER, operate in tandem. Program FLOW solves the flow equation and computes new pressures at the end of the time interval. These pressures and velocities computed from them, are used as input for program DISPER, which solves the convective-dispersion equation and calculates new concentrations. For operational simplicity program FLOW and DISPER are combined into a single program FFLOW.

The validity of the simulator has been tested with known exact and approximate analytical solutions for simplified cases. Program FLOW gives comparable results with the Theis equation and Program DISPER yields values reasonably matching the solutions for radial dispersion obtained by earlier investigators. Practical application of the simulator is demonstrated by applying it to hypothetical field problems.

The simulator could be used to analyze groundwater quality resulting from pumping or recharging of water from an aquifer having increased salt concentration with depth.

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ACKNOWLEDGEMENTS

The author wishes to thank his advisors, Professor R. A. Longenbaugh and Dr. J. W. N. Fead, for their encouragement, guidance and constructive comments. Thanks are also due to Dr. E. G. Thompson, Dr. D. W. Zachmann and Dr. D. B. McWhorter for the sound counsel, guidance and motivation provided by them during the period of development of this subject matter. The advice of Dr. D. K. Sunada, Dr. A. T. Corey, Dr. John Raich and Dr. A. Klute at different stages of this investigation is sincerely appreciated.

Sincere thanks are extended to Mrs. Diane English and Mr. John A. Brookman for their kind cooperation and effort in preparing the typed draft of this dissertation and to Mr. Shariatmadar Mahmood, Mr. V. P. Singh and Robert A. Chandler for day to day constructive discussions on the various aspects of this study.

The financial support provided by Colorado State University Experiment Station Project 110 and the computer money received from the Civil Engineering Department through unsponsered research funds, are thankfully achnowledged.

Last but not least, thanks are due to the author's family, Mrs. Chandrakanta, Manju and Ajay for the unlimited inspiration, exemplary cooperation and immense forebearance displayed by them through the periods of pessimism and optimism experienced in the process of accomplishment of this dissertation.

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CHAPTER I

INTRODUCTION

1.1 Description of the Problem

The ever expanding population of the world has placed greater-than-ever emphasis on the exploitation and utilization of ground water resources for the enhancement of agricultural production on one hand and for the extensive development of industrial and domestic water-supply systems on the other. Directly related to the development of ground water resources, is the common geological occurrence of fresh water aquifers underlain by salt water zones of varying depths. Due to indiscriminate ground water development, mostly through partially penetrating wells in such aquifers, during the last fifty years or so, their capacities to yield fresh water have been greatly impaired. As most of the aquifers of this type underlie highly developed urban and agricultural regions, their waters are subject to quality deterioration induced by the infiltration of liquid industrial wastes, irrigation return flows and incompletely treated domestic waste water.

Such situations are frequently encountered in aquifers extending along sea coasts of almost all the continents of the world, where salt water intrusion commences as a result of excessive pumping in the adjoining connected aquifers, but, the same are, by no means, confined to coastal aquifers alone. One of the largest and perhaps the most important non-coastal aquifer in the world viz. the Indus Basin in Pakistan falls under this category. Detailed accounts of the existence, nature, shape, slope and depths of fresh water - saline water interfaces for various types of aquifers have been given by Todd (1959), Davis and DeWeist (1966), Walton (1970), Feth (1970) and others.

Such aquifers are characterized by a vast number of special problems concerning the hydraulic engineer; the most important being the prediction of the rate of pumping at which a well of given penetration depth will discharge water having a salt concentration within the permissible limit for agricultural, industrial or domestic use. Intimately connected with the above is the assessment of the rate and extent of recoupment of fresh water or mixed quality of water when the pumping is stopped for a certain period and continued intermittently thereafter.

A problem somewhat analogous to the above, involving an oil-saturated region overlying a brine-saturated zone in a confined aquifer has been analyzed by Muskat (1949) who suggested a graphical procedure to solve the water coning problem beneath a partially penetrating oil well. This method has been adapted by Bennett et al. (1968) to study the upconing of saline water beneath a fresh water well. The problem of salt water - fresh water interface beneath a well has been studied by Wang (1965). This study purported to relate the discharge of a partially penetrating well to the well spacing, well penetration, well radius, aquifer thickness and fluid densities and to determine the optimum rate of fresh water production without entrainment of saline water, as a function of well geometry and aquifer characteristics. Experimental and numerical models for the movement of salt water cone in response to pumping by a partially penetrating well in a situation similar to the above have been constructed and studied by Sahni (1972) and Chandler (1973).

All these investigations assume the existence and persistence of a sharp interface between the fresh and salt water zones, as if the two were immiscible. Besides, the problem is treated as a steady-state case

of three-dimensional flow of incompressible fresh water over a static brine phase in radial coordinates, through non-deformable, isotropic and homogeneous porous media.

1.2 Purposes and Objectives.

In an actual field situation, the problem indicated in section 1.1 involves analysis of the non-uniform, non-steady movement of two miscible fluids of varying densities, viscosities and concentrations. The drawdown in the partially penetrating well causes radially symmetrical, three-dimensional, non-steady, non-uniform flow towards the well, which is governed by the mass-balance equation for water, hereafter called the 'flow equation' and the concentration gradient coupled with convection induces a transport of the solute towards the well governed by the convective-dispersion equation in radial coordinates.

The broad objective of this investigation is to find a solution to the above situation which will involve:

(i) Development of the appropriate flow equation for three-dimensional, non-steady, non-uniform flow of a compressible non-homogeneous fluid through elastic formations in a general system of coordinates.

(ii) Development of the appropriate convective-dispersion equation in tensorial form taking into account the tensorial nature of the dispersion coefficient. This will mean a combination of the mass-balance equation for the solute, Fick's law and an equation of state connecting the mass-density of the fluid at any point with the pressure and concentration at that point.

(iii) Development of a digital computer model simulator (taking advantage of radial symmetry to reduce the problem to a two

dimensional one) which seeks to solve the flow and convective-dispersion equations over the region of influence of the partially penetrating well.

(iv) Testing the validity of the simulator by comparison with available analytical, experimental or approximate solutions of simple cases.

CHAPTER II

REVIEW OF LITERATURE

2.1 Introduction.

As outlined in the previous chapter, this investigation involves the derivation and solution of the flow and convective-dispersion equations for a porous medium by the leap-frog technique. The flow equation, being an enunciation of the Eulerian mass-conservation principle coupled with Darcy's law for the unsteady flow of a non-homogeneous, compressible fluid through a non-reactive, isotropic and elastic porous medium, is one of the most well discussed topics in the literature connected with ground water movement; Jacob (1950), Hantush (1964), Davis and DeWeist (1966), Kochina (1949), Walton (1970), Bear (1972), Todd (1959), Harr (1962), Muskat (1946). Different forms of the flow equation suitable for different conditions have been arrived at by different investigators. As this principle of continuity has been in use in varied forms in almost all branches of science from the very early stages of development it is difficult to assign the credit for its development to any one individual. The flow equation appropriate to this study has been derived from first principles in Appendix A.

Unlike the flow equation, the convective-dispersion equation based on the concept of hydrodynamic dispersion through porous media is of a comparatively recent origin. Attempts made by investigators to explain the phenomenon of hydrodynamic dispersion have been multi-directional, varying from a purely theoretical analysis (mathematical or statistical) to experimental verifications and computer simulations. A chronological review of some of the important developments of this concept leading to the derivation and solutions of the convective-dispersion equation in

different forms is presented in the following paragraphs.

2.2 Conceptual and Analytical Developments.

According to Bear (1968), hydrodynamic dispersion is the macroscopic outcome of the actual movements of the individual tracer particles through the pores and the various physical and chemical phenomena that take place within the pores. Normally, two basic transport phenomena are involved in the process, a convective mass transport where the liquid moves along definite paths that may be averaged to yield streamlines and a process of molecular diffusion resulting from variations in tracer concentration within the liquid phase. Thus hydrodynamic dispersion is due to the combined action of both a purely mechanical phenomenon on a macroscopic scale (dispersion) and a physio-chemical phenomenon on a microscopic scale (molecular diffusion). The mathematical model of the phenomenon of hydrodynamic dispersion is a partial differential equation which is an expression for the mass-conservation of a tracer.

Fried and Combarnous (1971) define a tracer as a chemical compound dissolved in a fluid phase. The displacement of two miscible fluids may be considered as a tracer case when the fluids have the same densities and viscosities and there is no volume contraction by mixing. The terms coefficient of hydrodynamic dispersion, coefficient of dispersion, and coefficient of diffusion which are often used as measures of hydrodynamic dispersion may be defined as follows:

Let F_{t_i} = Total mass flux of the tracer carried by the fluid in direction i $[ML^{-2}T^{-1}]$.

F_{c_i} = Convective component of the mass flux of the tracer in direction i $[ML^{-2}T^{-1}]$.

J_i = Diffusive component of the mass flux of the tracer in direction i $[ML^{-2}T^{-1}]$.

$$F_{t_i} = F_{c_i} + J_i \quad . \tag{2.1}$$

On a macroscopic scale,

$$F_{c_i} = c\dot{v}_i + c\dot{v}_{oi} \tag{2.2}$$

where,

v_i = Average seepage velocity in direction i $[LT^{-1}]$.

$\dot{v}_{oi}$ = Fluctuations of the seepage velocity about the average in direction i $[LT^{-1}]$.

c = Concentration of the tracer in the fluid $[ML^{-3}]$.

$c\dot{v}_i$ = Flux carried by the average fluid motion.

$c\dot{v}_{oi}$ = Dispersive flux resulting from the velocity fluctuations about the mean.

Also by Fick's law of diffusion,

$$J_i = - D_d \cdot T_{ij} \cdot \nabla c \tag{2.3}$$

where; ∇c = Gradient of concentration.

D_d = Coefficient of molecular diffusion.

$\bar{T}_{ij}$ = Correction factor applied to the coefficient of molecular diffusion due to the tortuosity of the medium. It is a second rank tensor and is reciprocal of the tortuosity tensor as usually defined.

Therefore,

$$F_{t_i} = c\dot{v}_i + c\dot{v}_{oi} - D_d \cdot T_{ij} \cdot \nabla c \quad . \tag{2.4}$$

In analogy to Fick's law, it can be shown, Bear and Bachmat (1965, 1967),

that,

$$cv_{oi} = - D_{ij} \nabla c \quad , \tag{2.5}$$

where,

D_{ij} = Dispersion coefficient and is a second rank tensor.

Therefore,

$$F_{t_i} = cv_i - (D_{ij} + D_d T_{ij}) \cdot \nabla c$$
$$= cv_i - D^*_{ij} \nabla c \quad , \tag{2.6}$$

where,

$$D^*_{ij} = D_{ij} + D_d T_{ij} \tag{2.7}$$
$$= \text{Coefficient of hydrodynamic dispersion.}$$

One of the earliest observations of the phenomenon of hydrodynamic dispersion was made by Slichter (1905), who discovered that even in a uniform flow field the tracer advances in the direction of the flow in a pear-like shape that becomes longer and wider as it advances. He explained this by noting that the soil complex is composed of a large number of capillary tubes in each of which there is a velocity variation across the cross-section, which was responsible for the phenomenon he observed. Subsequently, around 1930, a zone of diffusion was observed at the salt water - fresh water interface in coastal aquifers which could not be explained by the prevalent immiscible fluid theory. This prompted the recognition of the dispersion process as a possible cause for the above phenomenon. This aspect was investigated both experimentally and theoretically by Kitagawa (1934) and later by Wentworth (1948) who postulated a 'rinsing theory' based on the hypothesis that the pores of the medium act as mixing cells filled alternately with salt and fresh water by the ocean waves. Danel (1952) used the capillary tube model and concluded

that dispersion was due to and depended upon the parabolic velocity distribution inside the capillaries. Following a similar approach, Taylor (1953, 1954) also came to the same conclusion and observed that in a capillary tube model, fluid particles initially on a plane perpendicular to the tube's axis, lie on a paraboloidal surface at any subsequent time and that the coefficient of dispersion for one-dimensional flow was proportional to the square of the average velocity.

With increasing research and interest in the phenomenon of dispersion, a notion developed among some investigators, that because of the discrepancy between the idealized medium of the mathematical models and the real medium, the mathematical models could not adequately describe the dispersion phenomenon. Accordingly, they focussed their attention towards the development of statistical models. Scheidegger (1954) employed the statistical theory of random walk in three dimensions and obtained a normal probability distribution for the displacement of a fluid particle in an isotropic porous medium. He neglected molecular diffusion and assumed an isotropic spread of the tracer with the result that his coefficient of dispersion turned out to be scalar with no distinction between the longitudinal and transversal directions. Further work on the scalar form of the coefficient of dispersion was done by Van Deamter, Brader and Lauweir (1955) who obtained a generalized solution of the dispersion equation for the capillary tube model.

For uni-directional flow and with a scalar coefficient of dispersion, Ebach and White (1958) presented an analytical solution to the simplified equation,

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D_L \frac{\partial^2 c}{\partial x^2} \qquad (2.8)$$

where the input concentration is a periodic function of time, u is the component of seepage velocity in the x-direction and D_L is the coefficient of longitudinal dispersion.

Scheidegger's finding of a scalar dispersion coefficient was, however, not supported by laboratory experiments which indicated a definite difference between the magnitudes of longitudinal and lateral dispersion. De Josselin de Jong (1958, 1958a) was perhaps the first to show by a statistical approach that the coefficient of the longitudinal dispersion D_L is about 5 to 7 times greater than the coefficient of lateral dispersion D_T and that both D_L and D_T are directly proportional to $\bar{v}$.

Rifai, Kaufman and Todd (1956) made a very comprehensive laboratory study to verify their theoretical work which was based on the capillary-tube and the disordered medium models and concluded that the dispersion coefficient in the direction of flow was nearly proportional to the first power of the average velocity. They derived the following equation for a three-dimensional case, assuming dispersion to be basically due to molecular diffusion and velocity convection, and neglecting the difference between the longitudinal and lateral dispersion coefficients:

$$\frac{\partial c}{\partial t} = D \nabla c - \text{div } (vc) \quad . \tag{2.9}$$

where,

D = coefficient of dispersion, and

v = component of seepage velocity.

Aris (1956) extended Taylor's analysis to straight tubes of any cross-section and showed that the effective coefficient of dispersion

could be obtained from the variance of the average concentration distribution caused by the phenomenon of dispersion. This was experimentally verified by Blackwell (1957). Following Wentworth's approach, Aris and Amundson (1957) also analyzed dispersion as a process of mixing in cells.

Based on further analysis of the dispersion coefficient, Scheidegger (1957, 1958) suggested two possible relationships:

(i) $$D \sim a'\bar{v}^2 \quad , \tag{2.10}$$

where a' is the dynamic dispersivity of the porous medium which is derived by a dynamic procedure applicable when there is enough time in each flow channel for appreciable mixing to take place by molecular transverse diffusion and $\bar{v}$ is the average seepage velocity.

(ii) $$D \sim a''\bar{v} \quad , \tag{2.11}$$

where a'' is the geometric dispersivity of the porous medium and is derived by a geometric procedure applicable where there is no appreciable molecular transverse diffusion from one stream line to another.

Further work on the dependence of dispersion coefficients on the mean velocity of flow was done by Ebach and White (1958) who suggested the following expression for the longitudinal dispersion coefficient D_L,

$$\frac{D_L}{\nu} = \alpha \left(\frac{vd}{\nu} \right)^{\beta} \tag{2.12}$$

where,

v = seepage velocity,

d = particle size of the medium,

ν = kinematic viscosity,

α = experimentally determined coefficient dependent on the properties of the porous medium

β = experimentally determined coefficient dependent on the flow regime.

Following a statistical approach similar to De Josselin de Jong, Saffman (1959) obtained the following expressions for D_L and D_T including the effect of molecular diffusion:

$$D_L = 1/2\ \bar{V}\ell s^2 \quad , \tag{2.13}$$

$$D_T = 2/16\ \bar{V}\ell \quad , \tag{2.14}$$

where,

$$s^2 = \text{Ln}\ \frac{3\ \bar{V}\ \tau_o}{\ell} - \frac{1}{12}$$

$$\tau_o = \ell^2/2\ D_d$$

ℓ = a characteristic length which is of the order of the grain size and depends on grain size distribution,

D_d = coefficient of molecular diffusion,

$\bar{V}$ = average Darcy velocity.

Another attempt in the same direction was by Blackwell, Rayne and Terry (1959) who obtained the following relationship between D_L and D_d ;

$$D_L/D_d = 8.8 \cdot P_e^{1.17} \quad \text{valid when} \quad P_e > 0.5 \quad , \tag{2.15}$$

where,

$$P_e = \text{Peclet number} = \frac{\ell\bar{V}}{D_d} \quad .$$

In a bid to obtain a more accurate inter-relation between the coefficient of molecular diffusion, and the longitudinal and lateral dispersion coefficients, Saffman (1960) extended his earlier work to cases where the Peclet number was of order unity, i.e. where molecular diffusion and macroscopic mixing were of the same order of magnitude.

Experimental and theoretical investigations on the dispersion phenomenon conducted prior to 1960, confirmed that the mere existence

of the porous medium and flow gives rise to a multi-component dispersion phenomenon. This tensorial character of the dispersion coefficient was experimentally verified by Bear (1961a). By theoretical analysis, he (1961b) showed that the dispersivity of a porous medium is a fourth rank tensor, which, in three dimensions, has 81 components (16 in two dimensions), out of which only 21 components (8 in two dimensions) are non-zero if the medium is isotropic. For an isotropic case, all these components depend on two essential constants which are the longitudinal and lateral constants of dispersion a_I and a_{II} respectively. Thus he deduced the following form for the dispersivity tensor $a_{ijk\ell}$ for an isotropic porous medium:

$$a_{ijk\ell} = \begin{bmatrix} a_I & a_{II} & 0 & 0 \\ a_{II} & a_I & 0 & 0 \\ 0 & 0 & (a_I - a_{II})/2 & (a_I - a_{II})/2 \\ 0 & 0 & (a_I - a_{II})/2 & (a_I - a_{II})/2 \end{bmatrix} \quad . \tag{2.16}$$

Extending this analysis to uniform flow in an isotropic medium, De Josselin de Jong and Bossen (1961) obtained the following expression for the coefficient of dispersion,

$$D_{k\ell} = a_{ijk\ell} \frac{v_i v_j}{v} \quad , \tag{2.17}$$

where, v_i and v_j are the components of the average velocity v in the i and j directions respectively.

Based on Bear's hypothesis that only that part of the velocity component was of significance, which was either parallel or normal to the mean flow direction, Scheidegger (1961) deduced a general form of

the dispersivity tensor in three dimensions having 36 independent non-zero components, which, for an isotropic case and for complete symmetry of the whole group of rotations, could be expressed by the following matrix:

$$a_{\alpha\beta} = \begin{bmatrix} a_{1111} & a_{1122} & a_{1122} & 0 & 0 & 0 \\ a_{1122} & a_{1111} & a_{1122} & 0 & 0 & 0 \\ a_{1122} & a_{1122} & a_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & a_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & a_{1212} \end{bmatrix} \qquad (2.18)$$

where,

$$a_{1212} = \tfrac{1}{2}\,(a_{1111} - a_{1122}) \qquad (2.19)$$

$a_{1111} = a_I$ and $a_{1122} = a_{II}$,

α represents the indices ij and β represents $k\ell$.

Thus he concluded that the dispersivity tensor given by Bear was a special case of this general dispersivity tensor. Writing in general form, Scheidegger's equation for geometric dispersivity of an isotropic medium becomes,

$$a_{ijk\ell} = a_{II}\,\delta_{ij}\,\delta_{k\ell} + \frac{a_I - a_{II}}{2}\,(\delta_{ik}\,\delta_{j\ell} + \delta_{i\ell}\,\delta_{jk}) \qquad (2.20)$$

where δ stands for Kronecker delta.

Thus,

$$D_{ij} = a_{II}\,v\,\delta_{ij} + (a_I - a_{II})\,v_i\,v_j/v \quad . \qquad (2.21)$$

Bachmat and Bear (1964) generalized these expressions for the curvilinear coordinate system as;

$$a_{ijk\ell} = \lambda\,g_{ij}\,g_{k\ell} + 2\mu\,g_{ik}\,g_{j\ell} \qquad (2.22)$$

and,

$$D_{ij} = \lambda\,g_{ij}\,v + 2\mu\,v_i v_j/v \quad . \qquad (2.23)$$

Also, they derived a general partial differential equation of hydrodynamic dispersion in a homogeneous, isotropic, porous medium in curvilinear coordinates as,

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial y^i} \left[|g|^{\frac{1}{2}} g^{ik} \left(\lambda v \frac{\partial c}{\partial y^k} + 2 \mu \frac{v_k v^1}{v} \frac{\partial c}{\partial y^\ell}\right)\right] - g^{ik} v_k \frac{\partial c}{\partial y^i} \tag{2.24}$$

which for an orthogonal system reduced to,

$$\frac{\partial c}{\partial t} = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial y^i} \left[\frac{h_1 h_2 h_3}{h_i^2} \left(\lambda v \frac{\partial c}{\partial y^i} + 2 \mu \frac{v_i v_k}{v h_k^2} \cdot \frac{\partial c}{\partial x^k}\right)\right] - \frac{v_i}{h_i^2} \frac{\partial c}{\partial y^i} \tag{2.25}$$

where,

g_{ij} = the fundamental tensor of the Reimanian space (a symmetric tensor of second rank) and the subscripts denote covariant components, such that,

g^{jk} = conjugate or reciprocal of g_{ij}, a second rank symmetric contra-variant tensor,

h_i = scale factors for the coordinate system, and,

λ and μ are invariants.

They derived general dispersion equations for plane two-dimensional flow in terms of Φ-Ψ coordinates from which equations for different particular cases could be easily obtained. Poreh (1965) obtained a similar expression for isotropic media as:

$$D_{ij} = A_1 \delta_{ij} + A_2 v_i v_j \tag{2.26}$$

where A_1 and A_2 are arbitrary functions of v^2 and the properties of the medium, fluid and tracer. From physical considerations he obtained different equations in dimensionless forms for low and high Reynolds numbers. Later, List and Brooks (1967) conducted a series of lateral

dispersion experiments and showed that for a given medium, the dynamic Peclet number vd/D_T is a function of any two of the following:

(i) Molecular Peclet number vd/D_d ,

(ii) Schmidt number ν/D_d ,

(iii) Reynold's number vd/ν .

They observed that for low Reynold's numbers, the lateral dispersion coefficient is independent of viscosity, i.e.,

$$D_T/vd = f\ (vd/D_d) \quad . \tag{2.27}$$

Further analytical work on the tensorial concept of dispersion was done by Whitaker (1967) who volume averaged the fundamental transport equation and obtained the following form for the coefficient of hydrodynamic dispersion D^*_{jk} for anisotropic media,

$$D^*_{jk} = D_{\alpha\beta}\ (\delta_{jk} + R\ B^I_{jk}) + A^I_{jik}\ v_i + A^{II}_{ji\ell k}\ v_i v_\ell \tag{2.28}$$

where,

$D_{\alpha\beta}$ = average molecular diffusivity,

A^I and A^{II} = symmetrical tensors bearing some functional relationship with the transport properties of the fluid,

R = a coefficient,

B^I_{jk} = tortuosity tensor.

For isotropic media, the third rank tensor term would be dropped and the expression becomes essentially the same as obtained by Bachmat and Bear.

Recently, Hunt (1973) analyzed the dispersion problem in a different manner and obtained the same expression for the coefficient of dispersion as was obtained by Bachmat and Bear (1964). A novel feature of his development was that he made only one assumption that the principal

directions of the dispersion tensor were respectively tangential and normal to the flow stream lines as against three assumptions used by Bachmat and Bear in their analysis (viz. $D_{k\ell} = a_{ijk\ell} \cdot v_i v_j / v$, $a_{ijk\ell} = a_{jik\ell}$, and $a_{ijk\ell}$ are invariant with respect to all coordinate rotations and reflections). Even this assumption has been verified by experiments.

With a view to analyze the effect of medium porosity on the longitudinal dispersion coefficient, Dagan (1967) used a Fourier Transform and perturbation analysis to conclude that D_L computed from the concentration profile decreased along a column of decreasing porosity in the direction of flow and vice-versa. Analytical solutions of some simplified idealized cases of the dispersion equation were developed by Ogata and Banks (1961), Ogata (1961), Harleman and Rumer (1962), Ogata (1964) and others. The same were later summarized and reviewed by Ogata (1970). But, since these cases have little, if any, practical importance, greater and greater attention has been given by investigators towards the development of numerical solutions of the generalized dispersion equation during the last few years.

2.3 Development of Numerical Techniques.

One of the first important works in this direction was by Douglas, Peaceman and Rachford (1959) who solved the problem of miscible displacement in a two-dimensional flow field using an alternating-direction implicit scheme. Later, Peaceman and Rachford (1962) used a weighting scheme for the convective terms at adjacent grid points in a centered-in-time finite difference analogue of the convective-dispersion equation and adopted the leap-frog technique of computing the pressure distribution at each time step from the flow equation, calculating the velocity

at each point from this pressure distribution and using these velocities to obtain the new concentration distribution at the next time step from the convective-dispersion equation. They demonstrated that the method worked well in one dimension. But, subsequent calculations with the method for two-dimensional miscible displacement with zero dispersivity produced the same results as were presented by them with non-zero dispersivities. This indicated that their method involved a numerical dispersion of the same order as the physical dispersion. Blair and Peaceman (1963) extended the work to include the effects of aquifer compressibility, but one of two difficulties was usually encountered: either the solution developed severe oscillations specially in the regions where the concentration changed rapidly or became smeared with numerical dispersion.

In a bid to tide over this difficulty, Stone and Brian (1963) developed a more sophisticated method which consisted of writing a general finite-difference equation for the one-dimensional convective-dispersion equation, containing arbitrary weightings of all the possible approximations to $\partial c/\partial x$ (space derivative of the concentration) and $\partial c/\partial t$ (time derivative of the concentration). This scheme involved six points for three adjacent space locations at two time levels and utilized the Crank-Nicolson (1947) approximation for the second space derivative $\partial^2 c/\partial x^2$. They also proposed an iterative scheme with three cycles per time step to improve the accuracy of the solution. With proper choice of weighting coefficients, this method did reduce oscillations and numerical dispersion but could not handle two- and three-dimensional problems and did not take the variations in density and viscosity into account.

With the primary object of reducing numerical dispersion, Garder, Peaceman and Pozzi (1964) successfully employed the method of characteristics (particle-in-cell method) for the solution of the convective-dispersion equation in two dimensions. The numerical procedure involved a stationary grid and a set of moving points to solve the characteristic equations of the convective-dispersion equation. Extensive testing in one dimension indicated that the method was accurate over a wide range of values of the dispersion coefficient, including zero and that increasing the number of moving points beyond two per grid did not significantly improve the accuracy of the solution. For a two-dimensional model, the method provided good agreement with observed values for low oil-solvent viscosity ratios, but failed to do so for high viscosity ratios. The method also did not take into account the tensorial nature of dispersion. According to Shamir and Harleman (1966) this method took much more computer time and storage than the Stone and Brian scheme for the same order of accuracy, except for the case where the coefficient of longitudinal dispersion was zero. However, the method was general and could be adapted to take the density and viscosity variations into account in a two-dimensional case.

Shamir and Harleman (1966) developed a very efficient method which took advantage of the Stone and Brian scheme by transforming the dispersion equation into Φ-Ψ (i.e., equipotential and stream lines) coordinates as,

$$\frac{\partial c}{\partial t} + q^2 \frac{\partial c}{\partial \Phi} = q^2 \frac{\partial}{\partial \Phi} \left[(a_I q + D_d) \frac{\partial c}{\partial \Phi} \right] + q^2 \frac{\partial}{\partial \Psi} \left[(a_{II} q + D_d) \frac{\partial c}{\partial \Psi} \right] \tag{2.29}$$

where,

q = seepage velocity along the stream line,

a_I = longitudinal dispersivity,

a_{II} = lateral dispersivity.

As the velocity was tangential to the Ψ = constant lines , there was only one convective term in this equation. This enabled the use of the Stone and Brian's weighting scheme for the convective and time terms without any modification. The dispersion at right angles to the direction of the velocity could be treated by the alternating-direction method. Once the convective term was treated correctly, superposition of the longitudinal and lateral dispersion on the convective solution yielded correct results. This method was found to be unconditionally stable and could be extended to three-dimensional problems without much difficulty. If the major axis of the dispersion tensor coincided with the velocity vector, the technique took into account the tensorial nature of the dispersion coefficient. For the case when the longitudinal dispersion was zero, the scheme displayed oscillations and it did not account for the variations in density and viscosity. For unsteady cases, its use was limited to only those situations where the stream lines and equipotentials did not shift position with time.

Hoppes and Harleman (1967a) developed the mass conservation equation for the tracer in a two-dimensional case and obtained an approximate analytical solution for a homogeneous, confined, isotropic aquifer under steady-state flow from a recharge well. The solution was verified with a numerical one and tested with experimental data. In extension of the above, Hoopes and Harleman (1967b) dealt with the problem of predicting temporal and spatial distributions of a tracer injected into

the steady flow between recharging and discharging wells of equal strength in an infinite, horizontal, confined aquifer. Approximate analytical solutions were obtained for various cases of the two-dimensional equation for mass conservation of the tracer in the Φ-Ψ coordinates and tested by comparisons with numerical solutions and experimental values.

Bruch and Street (1967) obtained a theoretical solution for two-dimensional, unsteady dispersion of a miscible fluid in an idealized, steady, one-dimensional flow through an isotropic porous medium. The results have been presented in terms of complementary error functions. The lateral and longitudinal dispersion coefficients were determined from a pair of steady-state dispersion experiments applied to two simplified mathematical models. With these values of the dispersion coefficients, the equations derived for the unsteady-state case were experimentally verified. It has been suggested that by transformation of the equation to Φ-Ψ coordinates, their results could be used for two-dimensional practical problems even with slightly converging or diverging stream lines.

Pinder and Cooper (1970) used the method of characteristics for the solution of the convective-dispersion equation and the iterative alternating-direction implicit scheme for the flow equation for numerical solution of the two-dimensional problem of transient salt water front. However, they assumed that the porosity, viscosity and dispersion coefficient were constant in time and space and that the dispersion coefficient was a scalar. Almost simultaneously, but independently, Reddell and Sunada (1970) developed flow and convective-dispersion equations for three-dimensional, non-homogeneous, unsteady flow fields

with density and viscosity variations between the two fluids, considering the tensorial nature of the dispersion coefficient in the Cartesian coordinate system. An implicit numerical technique was used to solve the flow equation and the method of characteristics with a tensor transformation was used to solve the convective-dispersion equation. The results from the flow equation were used in solving the dispersion equation and the results of the convective-dispersion equation were then used to solve the flow equation. This procedure was repeated over and over again following the so-called leap-frog technique. Because of the excessive storage required for information concerning each moving point, they used auxiliary storage in the form of a scratch tape. The results obtained displayed no over-shoot, under-shoot, or numerical dispersion. They, however, observed an erratic behaviour of the error when their model was tested for known solutions of one-dimensional cases, in as much as the error did not necessarily get smaller with smaller grid sizes. They proposed the trouble was due to the rough representation of straight boundary conditions by a series of rectangular or square grids. Another significant observation was a lag in the concentration profile resulting in a jerky frontal movement, when the same moving points remained inside a grid throughout a time step. This indicated that the method was sensitive to the number and relative position of the moving points in a particular grid at a given time level. These difficulties call for a better method for determining the average concentration in a grid.

Kraeger (1972) applied the method of Reddell and Sunada to a field problem and observed an artificial dispersion inherent in the method of characteristics which did not show up in Reddell and Sunada's analysis

due to the very small size of grids used by them. In the latter case, the effects of artificial dispersion were partially absorbed by the physical dispersion. Another difficulty encountered by her was a trial and error process to arrive at a time increment which produced a concentration distribution resembling the field situation. This rendered the method incapable of predicting reliable future concentration distributions. By hand calculations, she observed that use of distorted grids or different spacing of points in the x and y directions produced distorted concentration distributions, which further limited the use of the method for predictive purposes.

Bredehoeft and Pinder (1973) applied the method of characteristics and the iterative alternating-direction implicit technique, neglecting molecular diffusion and changes in density and viscosity, to the problem of aquifer contamination at Brunswick, Georgia with moderate success. Konikov and Bredehoeft (1973) applied the same technique to predict changes in dissolved solids concentration in response to spatially and temporally varying stresses in the Arkansas River Valley of south-eastern Colorado. They observed that the calculated changes in the concentration of dissolved solids were consistently less than the observed changes but that the relative increases from month to month tended to agree. These differences were attributed to either inaccurate or inadequate representation of the field situation by the numerical model. The scope of all these investigations was limited to uniform rectilinear flow of homogeneous fluids in a region which had no sources or sinks within it.

2.4 Applications of the Finite-Element Technique.

As seen from the preceding discussion of the various numerical methods, either the computer time or storage required for them becomes

prohibitive or else numerical or artificial dispersion tends to vitiate the results and at certain other times, the solution becomes severely oscillatory. These limitations, among others outlined above, focussed the attention of investigators towards the application of the finite element method to the solution of miscible displacement problems. The first attempt to apply this method to the solution of problems related to steady flow through anisotropic porous media was by Zienkiewicz, Mayer and Cheung (1966) followed by Taylor and Brown (1967) who extended the method to the solution of problems involving free surface. Price, Cavendish and Varga (1968) used the Galerkin method for solution of the one-dimensional diffusion-convection equation and showed that this method produced results of higher order accuracy and required less computer time than the central difference or non-central difference approximations as also the method of characteristics. They extended the finite-element method to the solution of two-dimensional problems.

Javandel and Witherspoon (1969) extended the use of the finite element method to the treatment of the flow equation for multi-layered aquifers of finite radial extent being pumped at constant rate through completely penetrating wells, using an iterative procedure to satisfy the constant discharge condition at the well boundary. They applied the method to flow towards partially penetrating wells also in multi-layered systems. Volker (1969) applied the method to the solution of steady free surface seepage problems through earth dams. Neuman and Witherspoon (1970) extended the technique further and successfully applied it to the problems of axi-symmetric flow from a circular pond in isotropic, homogeneous porous medium, axi-symmetric flow to a well in an unconfined aquifer, plane flow through a homogeneous dam, plane flow through a

homogeneous dam with a toe drain and the complex problem of a dam with a sloping core and a horizontal drain resting on a slightly permeable foundation whose bedding planes were inclined to the horizontal. They also devised a new iterative approach to obtain rapid convergence. Their method could handle cases where the free surface is discontinuous or where portions of the free surface are vertical or nearly vertical.

Guymon (1970a) applied the finite element method to the solution of the unsteady-state one-dimensional diffusion-convection equation and extended it (1970b) to the two-dimensional case taking both the longitudinal and lateral coefficients of dispersion into account but neglecting molecular diffusion. He indicated that the method could further be extended to the three-dimensional case as well. He, however, pointed out that the method is not, in general, applicable to problems defined by differential equations involving mixed partials and therefore neglected such terms in his solution.

Nalluswami (1971) improved upon the method followed by Guymon and included the mixed partial terms and the molecular diffusion component in his analysis. Hurr (1971) developed a finite-element ground water model that could solve problems connected with confined and unconfined flows for transient as well as steady-state conditions. Guymon (1972) suggested an improvement over his previous solution of the convective-dispersion equation, which displayed numerical dispersion and gave erratic results for small values of the dispersion parameters. This new approach did not make use of the exponential transformation developed in his earlier work. However, even this method did introduce slight errors for non-uniform flow cases and was not applicable to convection-dominated mass transport.

The scope of Guymon and Nalluswami's work was limited only to the solution of the two-dimensional simplified convective-dispersion equation in Cartesian coordinates. Simultaneous solution of the flow equation was not attempted by them. A serious limitation of the method was that it could not be applied to convection-dominant transports, which is the case for most field situations. The time-domain solution comprised of inherently explicit schemes and so exhibited convergence and stability problems. Although the need and criteria for an efficient element layout were indicated, yet they did not provide any scheme for automatic generation of such an element layout so as to give minimum band-width for the finite-element solution of the convective-dispersion equation. Such a scheme for efficient mesh generation, though quite important in the case of equal size element layout like the one used by Nalluswami and Guymon, is still more important in cases where the number of elements to be used is large and where due to substantial differences in concentration and potential gradients in different parts of the flow-domain, adoption of variable size elements becomes inevitable.

Another notable advancement towards the application of finite element method to solve three-dimensional steady-state and transient seepage problems was made by France, Parekh, Peters, and Taylor (1971) who introduced the concept of isoparametric elements to ensure higher oerders of accuracy in the solution. Later, Pinder and Frind (1972) applied the Galerkin method with curved isoparametric quadrilateral elements to the case of transient flow towards a well in an infinite aquifer and also to the case of flow towards a well in a leaky confined aquifer and compared the results so obtained with those available for the finite-difference method. Although, both the methods yielded results

of almost the same accuracy, the Galerkin procedure had more flexibility of application to a wide range of deterministic problems. Solution of the convective-dispersion equation was not attempted by these investigators.

Smith, Farraday and O'Connor (1973) compared the finite-element solutions of the two-dimensional diffusion-convection equation by the Rayleigh-Ritz and Galerkin methods and showed that the latter is more versatile in handling different types of boundary conditions and in solving problems like salt intrusion in long estuaries where the magnitude of the exponent used for transformation of the partial differential equation to a self-adjoint form is of the order of a few hundreds or more. The analysis was, however, limited to uniform rectilinear flow of homogeneous fluids in a region which had no sources or sinks within it.

Recently, Pinder (1973) used the Galerkin method, with curved isoparametric quadrilateral elements, to solve the two-dimensional groundwater flow and dispersion equations in cartesian coordinates and applied this mathematical model to simulate the movement of a plume of contaminated ground water on Long Island, New York. His results indicated that reasonably accurate simulation of the movement of contamination in the subsoil water can be obtained by the Galerkin-finite-element method. Solution in a radial flow field with well boundary was not attempted by him.

Desai (1973) developed a simplified and approximate finite-element solution of a linearized equation governing one-dimensional transient fluid flow such as occurs in the case of flow in and out of earthen banks with vertical faces. But, this method was limited only to situations that could be approximated as one-dimensional flow problems.

Neuman (1973) applied the Galerkin-finite-element formulation to the solution of saturated and unsaturated seepage problems and demonstrated that due to convenience in the treatment of prescribed flux boundary conditions in this method, handling of the seepage face is considerably simpler than the finite-difference techniques. This investigation did not cover miscible displacement problems.

2.5 Summary.

A review of the available literature on the subjects related to the present study indicates that finite difference and other numerical techniques developed by various investigators require prohibitive amounts of computer time and storage to solve the transient convective-dispersion equation with reasonable accuracy. Further, almost all the solutions exhibit numerical dispersion, artificial dispersion or severe oscillations in the results, or else require a not too well defined process of trial and error to arrive at the appropriate time increment for the solution to be reasonably good. Applications of the finite-element method have mostly been directed to the solution of the steady or unsteady flow equation with or without the free surface except the works of Guymon, Nalluswami, Smith et al., and Pinder. As stated before, the Rayleigh-Ritz approach of Guymon and Nalluswami is restrictive in practical applications.

The Galerkin approach of Smith et al. and Pinder does not have any such limitations. The latter, however, yields non-symmetric matrices, thus requiring larger computer time and storage. Both the approaches have been found to be comparatively free of numerical dispersion and oscillations and do not involve any uncertain trial and error procedures.

Besides these, the finite-element technique has the following additional advantages over other numerical methods:

(i) It can handle any irregular boundary configuration which may be discretized to triangular, quadrilateral or other isoparametric elements of any shape and size.

(ii) The method not only accommodates complex geometry and boundary conditions, but has also proved successful in representing various types of complicated material properties that are difficult to incorporate into other numerical methods. It is even possible to vary the properties within an element according to some preselected polynomial pattern.

(iii)Specified gradient boundary conditions are introduced naturally and with a better accuracy than in standardized finite difference procedures. This reduces the number of boundary conditions to be subsequently introduced into the matrices before solving them.

(iv) Higher order elements can also be conveniently used to improve accuracy without complicating the boundary conditions - a difficulty always arising with finite difference approximations of a higher order.

(v) As the finite-element formulation quite often results in a system of symmetric banded matrices, there is great ease and time-saving in solving them on a computer.

(vi) It can be conveniently extended to problems in higher dimensions.

(vii)Situations where the principal axes of the transmissibility or dispersivity tensors change in orientation may be conveniently handled by simple coordinate transformations in the finite-element

technique (Smith, et al. 1973). The same can not be easily modeled in a finite-difference approximation.

For self-adjoint problems, both the Rayleigh-Ritz and Galerkin finite-element formulations lead to identical systems of symmetric matrices. For non-self-adjoint problems, the latter results in non-symmetric matrices, whereas the former, almost always, yields symmetric matrices, provided the corresponding variational functional exists. In certain cases, like the one analyzed by Guymon and Nalluswami with the Rayleigh-Ritz formulation, the transformation variable required to transform the system to a slef-adjoint form may pose computational problems. For certain other situations, the presence of higher order derivatives in the weighted-residual of the Galerkin approach may create insurmountable difficulties with regard to higher order continuities. A judicious choice between the two approaches has, therefore, to be made depending upon the problem under investigation.

2.6 Further Definition of Problem.

With this background about the performance of the various solution techniques, it is proposed to use the finite-element method for the simultaneous solution of the flow and convective-dispersion equations applicable to the situation under study. This investigation would, thus, include the following:

1. Development of the general flow equation for an isothermal, three-dimensional flow field where the porous medium is deformable and isotropic and the fluid is compressible and non-homogeneous with regard to density and reduction of such a flow equation to the case of an axisymmetric flow towards a well.

2. Development of the general convective-dispersion equation for an isothermal three-dimensional case in an isotropic mdeium taking molecular diffusion and the tnesorial form of the dispersion coefficient into account assuming isotropic dispersivity and a non-reactive tracer and reduction of such an equation to the case of an axisymmetric flow towards a well.

3. Finite-element formulations for the transient flow and convective-dispersion equations.

4. Development of an efficient scheme for automatic mesh generation for the simultaneous solution of the flow and convective-dispersion equations by the finite-element method for the field situation of axisymmetric flow towards a partially penetrating well.

5. Development of a scheme for handling the different boundary conditions for the flow and convective dispersion equations for the case of confined, axisymmetric, unsteady flow towards a partially penetrating well.

6. Development of a computer program for simultaneous solution of the flow and convective-dispersion equations by an implicit leap-frog technique, testing the program by comparison with other known solutions and finally applying the same towards the solution of field problems.

CHAPTER III

MATHEMATICAL MODEL AND NUMERICAL SIMULATOR

3.1 Development of the flow equation.

As explained earlier, the flow equation is a combination of the principle of conservation of mass expressed from the Eulerian viewpoint of fluid motion and the generalized form of Darcy's law for non-homogeneous fluids. The principle of conservation of mass as explained in Appendix A is based on the following assumptions:

(i) The size of the volume-element over which the mass-balance is considered does not vary with time.

(ii) There are no chemical reactions going on in the system and there are no sources or sinks.

(iii)There is only one non-reactive tracer present in the system.

(iv) The relationship between the fluid-density, pressure and concentration can be expressed by a first order equation of state and the proportionality factors are independent of pressure and fluid-composition.

(v) There is no change in volume upon mixing of fluids of different ionic concentrations.

With these limitations, the mass-balance may be expressed in compact tensorial notation as follows:

$$(\phi S)_t + \frac{1}{\sqrt{g}} \left(\sqrt{g} \frac{q_i}{h_i^2} \right)_{,i} = - \frac{\phi S}{\rho} \rho_t - \frac{q_i}{\rho h_i^2} \rho_{,i} \qquad (3\text{-}1)$$

where,

ϕ = Porosity of the porous medium.

S = Saturation of the porous medium.

q_i = Macroscopic flow velocity in i direction.

ρ = Mass density of the fluid.

g = Absolute value of the determinant of the metric tensor.

h_i = Scales of coordinate transformation. $i=1,2,3$.

For the general case of an anisotropic, non-homogeneous porous medium and for a fluid, non-homogeneous with respect to density, Darcy's law may be stated as, Happen and Brenner (1965); Yih (1961):

$$q_i = v_i \phi S = - \frac{k_i k_r}{\mu} \left(\frac{1}{h_i} P_{x_i} + \rho g \, z_{x_i} \right) \qquad (3\text{-}2)$$

where, the subscript x_i denotes derivative with respect to X_i .

v_i = Seepage velocity component in i direction.

k_i = Absolute permeability in i direction at complete saturation.

k_r = Relative permeability at saturation S .

P = Fluid pressure.

Assuming that,

(i) Darcy's law holds for the flow situation under study,

(ii) there is no contribution to flow due to thermo-dynamic and adsorptive force gradients or due to electric charges carried by wet soil particles,

(iii) k_i and k_r are independent of pressure, temperature and concentration,

(iv) a linear relationship exists between the porosity and pressure,

(v) the medium is isotropic,

and combining equations 3-1 and 3-2 as elaborated in Appendix A,

$$\frac{1}{\sqrt{g}}\left[\frac{\sqrt{g}}{h_i^2}\left\{\frac{k_i k_r}{\mu}\left(\frac{1}{h_i}P_{x_i}+\frac{\rho g}{h_i}z_{x_i}\right)\right\}\right]_{,i}+\frac{1}{\rho h_i^2}\rho_{,i}\cdot$$

$$\left\{\frac{k_i k_r}{\mu}\left(\frac{1}{h_i}P_{x_i}+\frac{\rho g}{h_i}z_{x_i}\right)\right\}=\left[\rho_o\phi_o S\,(\beta+C_F)\,P_t+\alpha\phi_o SC_t\right]\cdot\frac{1}{\rho}\quad . \tag{3-3}$$

For radial flow towards a partially penetrating well in a saturated medium, equation 3-3 reduces to the following approximate relationship,

$$\frac{1}{r}\left[\left\{\frac{\rho rk}{\mu}\left(P_r+\rho g\,z_r\right)\right\}_r+\left\{\frac{\rho rk}{\mu}\left(P_z+\rho g\right)\right\}_z\right]=$$
$$\rho_o\phi_o\,(\beta+C_F)\,P_t+\alpha\phi_o\,C_t\quad . \tag{3-4}$$

For the problem under investigation, the assumption of the validity of Darcy's law is as much justified as it is for any other problem in well-hydraulics. No doubt, there will often be a small zone of non-linear flow in close proximity to the well where refinements to Darcy's law are warranted Ahmad (1967): Ahmad and Sunada (1969). However, such refinements are not considered necessary in the present investigation in view of the fact that minor approximations, thus introduced in a very small portion of the flow region, will not appreciably affect the total salt transport due to hydrodynamic dispersion and convection. The assumption that the contribution to flow due to thermodynamic gradient is small, is justified by the fact that temperature variations of the subsoil in any particular saturated region are generally small and past researchers have indicated that the quantum of thermal-gradient-actuated flow in a saturated soil is rather small as compared to that actuated by the mechanical gradient; Gurr, Marshall and Hutton (1952); Hadley and Eisenstadt (1955); Habib and Soerio (1957); Kuzmak and Serada (1958);

Rollins, Spangler and Kirkham (1954). The effect of electrical charges carried by wet soil particles and adsorptive force gradients is even less, Hillel (1971).

The assumption regarding the invariance of absolute and relative permeabilities with changes in pressure and concentration is justified by the observation that in naturally occurring saturated aquifers under isothermal conditions, there is hardly any effect of pressure or concentration on permeability so long as the fluid behaves as a continuum and the concentration remains small. The linear relationships between porosity and pressure and between the density, pressure and concentration used in the derivation of flow-equation in Appendix A, though not rigorously true, have often been used with success by earlier investigators Reddell and Sunada (1970); Breittenbach (1968). Under isothermal conditions, contribution to flow due to reactions between soil, water and ordinary salts is very small and so the reaction, production or consumption terms in the flow-equation may be omitted without introducing appreciable errors. By observations in physical chemistry, it is also known that there is little change in the volume of a solution upon mixing of fluids of different ionic concentration, Bredehoeft and Pinder (1973).

The only assumption made in Appendix A, that is questionable for a field situation, is that of the isotropy of the medium. This has been introduced in this study to avoid complex tensorial expressions for the coefficients of dispersion as explained in Chapter II. This analysis, based on the assumption of an isotropic medium, will, however, not apply to a flow region which is highly anisotropic.

3.2 Development of the Convective Dispersion Equation.

As discussed in Appendix B, the convective-dispersion equation is a combination of the mass-balance equation for the tracer and Fick's law of diffusion. The resulting equation in tensorial form is reproduced below.

$$C_t = \frac{\rho}{\rho-\alpha C} \cdot \frac{1}{\phi\sqrt{g}} \left[\frac{\sqrt{g}\phi}{h_i^2} \left\{ \lambda V C_{,i} + \frac{2\mu v_i v_j}{V h_j^2} C_{,j} + D_d T C_{,i} \right\} \right]_{,i} - \frac{v_i}{h_i^2} C_{,i} \qquad (3\text{-}5)$$

where, $,i$ = covariant derivative,

C = concentration,

α = proportionality factor as defined in Appendix A,

$\lambda = a_{II}$ = lateral dispersivity of the medium,

V = absolute velocity of the fluid,

$\mu = (a_I - a_{II})/2$,

a_I = longitudinal dispersivity of the medium,

D_d = coefficient of molecular diffusion,

T = tortuosity.

For axi-symmetric flow towards a partially penetrating well, equation 3.5 reduces to,

$$C_t = \frac{\rho}{\rho-\alpha C} \left[\frac{1}{\phi r} \left\{ \phi r \left(D^*_{11} C_r + D^*_{12} C_z \right) \right\}_r + \frac{1}{\phi} \left\{ \phi \left(D^*_{22} C_z + D^*_{12} C_r \right) \right\}_z \right] - u C_r - v C_z \qquad (3.6)$$

where,

$$D^*_{11} = \lambda V + 2\mu \frac{u^2}{V^2} + D_d T \quad ,$$

$$= D_T + (D_L - D_T) \frac{u^2}{V^2} + D_d T \quad ,$$

$$D^*_{22} = \lambda V + 2\mu \frac{v^2}{V^2} + D_d T \quad ,$$

$$= D_T + (D_L - D_T) \frac{v^2}{V^2} + D_d T \quad ,$$

$$D^*_{12} = D^*_{21} = 2\mu \frac{uv}{V^2} + D_d T \quad ,$$

$$= (D_L - D_T) \frac{uv}{V^2} \quad ,$$

$D_T = a_{II} V$ = coefficient of lateral dispersion,

$D_L = a_I V$ = coefficient of longitudinal dispersion,

u and v are radial and vertical components of velocity.

The various assumptions inherent in the development of the above equation are:

(i) Fick's law is applicable.

(ii) There is no production or consumption of the tracer due to chemical reactions.

(iii) The medium is isotropic so that dispersion coefficients D_T and D_L could be defined as above and the tortuosity tensor T is a scalar.

All these assumptions are reasonable for a dilute solution of an inert tracer under isothermal state, Crank (1956), which is the case for the situation under study. Limitations of the assumption of isotropy have already been indicated in the previous section. The main advantage of this assumption is that the dispersivity tensor $a_{ij\ell m}$, which is of rank four, reduces to only two terms, a_I and a_{II} (longitudinal and lateral dispersivities) for an isotropic porous medium.

3.3 The Finite-Element Method.

As outlined in Chapter II, finite-element approximation for any tractable problem could be obtained either by an adaptation of the Rayleigh-Ritz technique of variational calculus, which requires a variational functional, physically representing the rate at which energy is being dissipated per unit volume or weight of the fluid, to be minimized over the entire flow domain; or by using weighted residual techniques like the Galerkin method, which preclude the necessity of developing a variational functional for the problem. The Rayleigh-Ritz method is the most widely accepted means of arriving at the finite element representation of a problem. In addition to the numerous merits pointed out by Guymon (1970b), it admits less restrictive approximating functions and the conditions of convergence for this method have been well established, Tottehnam and Brebbia (1970).

The fact that a variational functional may not exist for a wide variety of problems or may be too complicated to handle by readily available numerical shcemes, does impose a limitation on its use. On the other hand, owing to the direct occurrence of the differential operators of the governing equation of the problem into the integrals involved in the Galerkin method, a higher order of continuity may have to be guaranteed by the shape function in order to avoid inter-element contributions. This restriction on the choice of shape functions may sometimes pose insurmountable difficulties, Zienkiewicz (1971).

In the formulation presented in this chapter both the approaches have been discussed in relation to the problem under study. Both these formulations are based on the inherent assumption that within each

element, the variables H (defined in section 3.5) and C are uniquely represented by a polynomial, continuous at the element boundaries. This assumption is justified within the limits of accuracy of the Weierstrass approximation theorem, Courant and Hilbert (1963) which states that a function $H(x_1,x_2,x_3,.....x_n)$ or $C(x_1,x_2,x_3,.....x_n)$, which, along with its derivatives up to the k^{th} order, is continuous in the closed region $a_i \leq x_i \leq b_i$, may be uniformly approximated by polynomials in this interval in such a way that the derivatives of H or C up to the k^{th} order are also approximated uniformly by the corresponding derivatives of the polynomials.

Rigorous cirteria for selecting the order of the polynomial representing these variables H or C are completeness, compatibility and independence of the pattern from the orientation of the local coordinate system. The requirement of completeness implies that over the region of application of the polynomial, there should exist combinations of values of the generalized coordinates that cause all points on an element to experience the same pressure or concentration. A polynomial with a constant term in it might take care of this requirement. The compatibility requirement implies that there should be no discontinuities of pressure or concentration within an element and between adjacent elements. Since polynomial models are inherently continuous, continuity within the element is ensured by the choice of any polynomial.

The condition of interfacial compatibility is satisfied if;

(i) the same polynomial model is used for all the elements,

(ii) the pressure or concentration values along any interface

depend on the nodal-point values pertaining to that interface only, (iii)inter-element nodal compatibility is ensured.

It may be shown, Desai and Abel (1972), that polynomial models do satisfy requirements (i) and (ii) and that requirement (iii) is implied in the usual assembly procedure of the finite-element method.

As the differential operators in the governing equations 3.4 and 3.6 happen to be of the second order, prima facie, it appears that second order continuity has to be guaranteed by the shape function for the Galerkin method, but as has been shown later, use of the divergence theorem reduces the order of these differentials to one and thus obviates the requirement of second order continuity. For both the approaches in this study, although higher order shape functions might add to accuracy, only linear polynomials have been considered, on the presumption that other approximations implicit in the analysis would far offset the improved accuracy attained by adopting more complex polynomial representations of the functions H or C. Following a similar reasoning, although, as indicated in Chapter II, isoparametric elements could be used, yet, in this investigation, where the scope is limited to simpler boundary configurations, triangular elements have been considered adequate.

Since, as explained above, the pressure or concentration varies linearly along any side of a triangular element, the same pressure or concentration is bound to exist all along an interface, if identical pressures or concentrations are imposed at the nodes. Thus the pressure or concentration distribution functions automatically guarantee continuity of pressure or concentration with adjacent elements. However, there may be discontinuities in the first derivative of the pressure or

concentration parameters between adjacent elements. To minimize the effects of such discontinuities, it is necessary to use smaller elements in areas of rapid changes in the first derivatives of pressure or concentration, while larger elements may be adequate for comparatively insensitive regions.

Once continuity between adjacent elements is ensured, the Galerkin method would consist of choosing a continuous weighting function which might be the shape function itself, and equating the element by element weighted residuals to zero. On the other hand, the Rayleigh-Ritz method would consist of minimization of the variational functional over the entire flow region. That this is a true minimizing or stationarity principle can be mathematically proved, Kantorovich and Krylov (1958) and that this minimization process implies solution of the flow or convective-dispersion equation can be shown by using the fundamental lemma of calculus of variations.

The linear models discussed above, satisfy the last criterion of independence of the pattern from the orientation of the local coordinate system also. This aspect has been elaborated in detail by Desai and Abel (1972) and Dune (1948). This property of the model is known as geometric isotropy, spatial isotropy or geometric invarience.

3.4 Mesh Layout.

Once the element shape and degree of polynomial approximating the function H or C has been finalized, the next step is to figure out an element layout covering the flow domain. Taking advantage of radial symmetry and assuming that the contribution of the nearly spherical and non-radial flow towards the bottom of a partially penetrating well, Muskat (1946) is negligible, the three-dimensional flow problem may be

reduced to one that could be studied on a two-dimensional region in the r-z plane typified by a vertical cross-section of the aquifer passing through the axis of the well. Even on this cross-section, only one-half portion lying towards any one side of the well-axis would be adequately representative of the flow system as far as this investigation is concerned. Therefore, it is this two-dimensional region, that has been sub-divided into a mesh of triangular finite elements, not necessarily congruent or symmetric. For a general case, the tirangular elements would comprise an assortment of acute angle, right angle and obtuse angle triangles with few, if any, of their sides parallel or perpendicular to the coordinate axes. For such cases, closed form expressions for higher moments over the elemental area, although possible to derive, would become rather complex and tedious. It is, therefore, desirable to use the Gauss-quadrature approximation as suggested by Zienkiewicz (1971).

As explained in Section 3.3, the element layout is to be arranged in such a way that the regions of maximum pressure or concentration gradients are covered by smaller size elements. Thus, smaller elements have to be provided in the vicinity of the well, with the sizes gradually increasing with distances from the well both in r and z directions, so that abrupt changes in element sizes are avoided. Another important requisite for the mesh layout stems from the point of view of computational efficiency. It is well known that finite element formulation of the flow or dispersion equation would result in the formation of banded matrices, with the band-width given by the following rules:

(i) For symmetric matrices, band-width = IBAND = Maximum of the differences in the numbers assigned to any two adjacent nodal points in the entire mesh layout plus one.

(ii) For unsymmetric matrices, band-width = twice the maximum of the differences in the humbers assigned to any two adjacent nodal points in the entire mesh layout plus one.

Thus, there is a certain mesh layout with a certain numbering scheme for the nodal points and elements that will give the smallest possible band width.

An indication of the boundary orientation for an efficient element layout for simple flow regions has been given by Guymon (1970b). However, he did not develop any mesh-generation shceme for a suitable element layout. In this investigation, a computer program has been developed[1] for automatic mesh-generation, based on the algorithm of Zienkiewicz and Phillips (1971). As discussed in Chapter IV, this program requires the flow region to be divided into one or more loops depending upon the variations in element sizes. Each loop is divided into a number of quadrilaterals and the shorter diagonal of each quadrilateral is joined to produce a triangular element layout. For multi-loop regions, this program incorporates an optimization scheme, Collins (1973), to renumber all the nodes in the mesh so as to yield a minimum band-width. Data requirement for this program consists of the coordinates of eight points delineating the boundary geometry of each loop taken in an anti-clockwise sense, the number of divisions into which each side is to be divided and the maximum and minimum values of the r and z cordinates for each loop. In addition, information regarding the common sides between any two loops has also to be provided as input in the form of an array as

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[1] With the cooperation of Dr. E. G. Thompson, Civil Engineering Dept., Colorado State University.

explained in Appendix G. The output comprises a film plot of the layout and a deck of punched cards giving the coordinates of all the nodes and assigned numbers of all the nodes and elements.

3.5 Finite Element Formulation for the Flow Equation.

With a view to transform equation 3.4 to a tractable form, it is expedient to introduce two terms of negligibly small magnitudes viz. $gz\,\rho_r$ and $gz\,\rho_z$ and modify it as follows:

$$\rho_o\phi_o\,(\beta+C_F)\,P_t + \alpha\phi_o C_t \cong \frac{1}{r}\cdot\frac{\rho k}{\mu}\{P_r + \rho g z_r + gz\,\rho_r\}$$

$$+\left\{\frac{\rho k}{\mu}\,(P_r + \rho g z_r + gz\,\rho_r)\right\}_r + \left\{\frac{\rho k}{\mu}\,(P_z + \rho g + gz\,\rho_z)\right\}_z \qquad (3.7)$$

where the subscripts r , z and t denote derivatives with respect to them. Setting,

$$\rho_o\phi_o\,(\beta+C_F) = E$$

$$\alpha\phi_o = F$$

$$P + \rho gz = H$$

$$\frac{\rho k}{\mu} = S$$

$$EP + FC = Y$$

equation 3.7 reduces to,

$$Y_t = \frac{1}{r}\,(r\,S\,H_r)_r + (SH_z)_z \qquad . \qquad (3.8)$$

The Galerkin Approach. Following the Galerkin technique as discussed in Appendix C with an arbitrary weighting function W_p where p=i,j,k and applying divergence theorem to the weighted residual, with a view to reduce the order of differentials occurring in it, the following equation is obtained:

$$\iint_V [S\, H_r\, (W_p)_r + S H_z\, (W_p)_z + W_p\, Y_t\,]\, r\, dr\, dz = \int_S W_p\, S H_r\, n^1\, dS$$

$$+ \int_S W_p\, S H_z\, n^3\, dS \quad . \tag{3.9}$$

Using the boundary conditions discussed in Section 3.7, the R.H.S. of equation 3.9 reduces to zero except for the well face and the constant head boundaries. For the well boundary, value of the expression on the R.H.S. is known in terms of the flow rate q and for the constant head boundaries, this expression may be set equal to some unknown value $[R]$. It is shown in Section 3.7 that, in view of the known values of H on the constant head boundaries, the value of $[R]$ is not required to be computed for the solution of the resulting system of simultaneous equations.

Substituting the above values on the R.H.S. of equation 3.9 and transforming it to a local coordinate system referred to the centroid of the element as the origin, the following system of equations is obtained,

$$\iint_{R^m} [S\, H_\xi\, (W_p)_\xi + S\, H_\eta\, (W_p)_\eta + W_p\, Y_t] \, (\bar{r}^m + \xi)\, d\xi\, d\eta =$$

$$\int_{S_2^m} W_p\, \rho q\, r_w\, d\eta + [R] \tag{3.10}$$

where, the subscripts ξ, η and t denote derivatives with respect to ξ, η and t,

$$\xi = r - \bar{r}^m$$

$$\eta = z - \bar{z}^m \quad .$$

$\bar{r}^m$ and $\bar{z}^m$ are the global coordinates of the centroid and $\bar{R}^m$ and $\bar{S}_2^m$ respectively refer to the area and the portion of the well-face, if any, covered by the boundary of the m^{th} element.

Defining a continuous shape function [A] as explained in Appendix C, such that,

$$H = [A] \{H\}^m$$

where the matrix $\{H\}^m$ refers to nodal point values of H for the m^{th} element and assuming that this shape function itself is the weighting function, equation 3.10 yields,

$$\iint_{R^m} ([S\ [A]_\xi\ (A_b)_\xi + S\ [A]_\eta\ (A_b)_\eta]\ \{H\}^m + A_b\ [A]\ \{Y_t\}^m)$$

$$(\bar{r}^m+\xi)\ d\xi\ d\eta = \int_{S_2^m} A_b\ \rho q\ r_w\ d\eta + [R] \quad . \tag{3.11}$$

Evaluating the differentials and integrals and writing the system in the symbolic form defined in Appendix C, equation 3.11 may be written as,

$$[FSL]\ \{H\}^m + [FPLE]\ \{Y_t\}^m = [Q]^m + [R]^m \quad . \tag{3.12}$$

Following the general process of assembly applicable to finite element formulations for combining equations similar to 3.12 for all the elements in the layout, the following system of simultaneous equations is obtained,

$$[SK]\ \{H\} + [PK]\ \{Y_t\} = [QK] + [R] \quad . \tag{3.13}$$

The Rayleigh-Ritz Approach. Following the alternative Rayleigh-Ritz technique, the variational principle for equation 3.8 may be verified to be, Hildebrand (1965),

$$J = \iint_R \left[\frac{S}{2} (H_r)^2 + \frac{S}{2} (H_z)^2 + H Y_t \right] r \, dr \, dz - \int_{S_2} \rho q \, r_w \, H \, dz \quad . \tag{3.14}$$

Equating the first variation of J to zero, it may be shown that the natural, geometric and well boundary conditions are included in this variational principle. Its transformed form written for the m^{th} element in terms of local coordinates is,

$$J^m = \iint_{R^m} \left[\frac{S}{2} \{ (H_\xi)^2 + (H_\eta)^2 \} + H Y_t \right] (\bar{r}^m + \xi) \, d\xi \, d\eta - \int_{S_2^m} \rho q \, r_w \, H \, d\eta \tag{3.15}$$

The minimization process for this functional, J, consists of evaluating the contributions from all the nodes in the layout to the differentials $J^m_{H_p}$ $(p=i,j,k)$ for each element, summing the relevant contributions for each node and equating the sum to zero for stationarity. This process for the m^{th} element yields,

$$J^m_{H_p} = \iint_{R^m} \left[S \, H_\xi \, (H_\xi)_{H_p} + S \, H_\eta \, (H_\eta)_{H_p} + Y_t \, H_{H_p} \right] (\bar{r}^m + \xi) \, d\xi \, d\eta$$

$$- \int_{S^m} (r_w \, \rho q \, H)_{H_p} \, d\eta = 0 \quad , \tag{3.16}$$

where the subscript H_p denotes a derivative with respect to H_p. Equation 3.16 may be verified to be the same as equation 3.11 except for the unknown terms $[R]$ which do not affect the solution at all. Thus, so far as the flow equation 3.8 is concerned, which is already in the self-adjoint form, Hildebrand (1965), both the Galerkin and Rayleigh-Ritz techniques lead exactly to the same system of simultaneous equations 3.13.

3.6 Time Domain Formulation of the Flow Equation.

As discussed in Section 3.5, the finite element formulation of equation 3.8 yields,

$$[PK] \{Y_t\} = [QK] + [R] - [SK] \{H\} \quad .$$

Time domain solution of this system may be obtained in several ways, viz. by the methods of undetermined parameters (collocation, subdomain, Galerkin or least squares) as outlined by Crandall (1956) or by combining the usual integration schemes Runge-Kutta and Adams-Moulton, etc., Nalluswami (1971), Guymon (1970b). The latter approach is time consuming, requires extra computer storage and has been found to cause stability and convergence problems unless the time step chosen is very small. The shortcuts suggested, Robert G. Baca (1973)[1], to expedite convergence of the scheme are not applicable to a general system of equations. Unlike the case of a single first order equation, Gerald Curtis (1970), it is extremely difficult to develop criteria for the convergence of successive recorrections by the Adams-Bashford corrector for a system of equations. It is even more difficult, in any particular case, to know whether such criteria, if available, are actually satisfied or not. Therefore, most authors, Conte (1965), Peter Henrici (1965), caution against the use of the corrector more than once and recommend to restart from the Runge-Kutta onwards at every change of the time-step, which is a time consuming process. In the present study both the undetermined parameters and Adams-Moulton methods were tried and finally, to retain simplicity without substantial loss of accuracy, the Galerkin method of weighted residuals has been adopted. For the Galerkin method developed in Appendix C, the equation residual for the time-domain solution gives,

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[1] By personal communication with Robert G. Baca, 1973, Pac. NW Labs..

$$\int_{o}^{\Delta t} N_1 \left[[PK] \{Y_t\} + [SK] \{H\} - [QK] - [R] \right] dt = 0 \quad . \quad (3.17)$$

In similarity to the finite-element discretization in space, assuming a linear interpolation of H in the time-domain for a small time interval Δt ,

$$\{H\} = [N] \begin{Bmatrix} \{H\}_o \\ \{H\}_1 \end{Bmatrix} \quad (3.18)$$

where,

$[N] = [\, N_o \quad N_1 \,] = [\, 1 - \frac{t}{\Delta t} \quad \frac{t}{\Delta t} \,]$

$\{H\}_o$ = nodal point values of H at $t=0$.

$\{H\}_1$ = nodal point values of H at $t=\Delta t$.

As for the formulation in space, higher order polynomials with more elaborate elements may be tried for the time domain solution if the accuracy desired warrants, Zienkiewicz (1971). For the present study, results obtained by the linear relationship of equation 3.18 are considered adequate and therefore, the time-domain formulation is based on this linear relationship.

Since,

$$Y_o = E\,(H_o - \rho_o g z) + F\,C_o \quad , \quad (3.19)$$

it follows that within the approximation inherent in the leap-frog technique,

$$Y_1 \simeq E\,(H_1 - \rho_o g z) + F\,C_o \quad , \quad (3.20)$$

and,

$$Y_t \simeq E \cdot H_t \quad (3.21)$$

where the subscripts o and 1 refer to the time levels $t=0$ and $t=\Delta t$ respectively.

Substitution of equation 3.21 into 3.17 and integration of the latter yields,

$$\left[[PK] \frac{E}{\Delta t} + \frac{2}{3} [SK] \right] \{H\}_1 = [QK] + [R] + \left[[PK] \frac{E}{\Delta t} - \frac{1}{3} [SK] \right] \{H\}_o \tag{3.22}$$

which is the required recurrence relation for the time-domain solution. A similar recurrence relation may be obtained by following the subdomain method as explained in Appendix C.

3.7 Treatment of Boundary and Initial Conditions for the Flow Equation.

To start with, values of ϕ , ρ , C and H for each node are prescribed as initial conditions, say,

$\phi_o(r,z)$, $\rho_o(r,z)$, $C_o(r,z)$, $H_o(r,z)$ at t=0 .

Besides these initial conditions, there will, in general, be three types of boundary conditions:

(i) Natural or reflective boundary conditions which specify that $H_n = 0$, on a portion of the exterior boundary, n being normal to the boundary surface drawn in an outward sense. The subscript n denotes a derivative with respect to n . Such boundary conditions apply to all impermeable or no-flow boundaries. As shown in Appendix C, the finite element formulation, in itself, implies satisfaction of such boundary conditions.

(ii) Geometric boundary conditions which specify the values of H on a portion of the boundary. At a section of the aquifer, beyond the radius of influence, r_o of the well, or at a large depth below the bottom of the well, H will remain unchanged for all time periods and so, will be represented by specified values such as,

$H_1(r,z)$, $H_2(r,z)$,....., $H_n(r,z)$ $\forall$ $t \geq 0$.

A convenient device that has been adopted in the computer program, to take such geometric boundary conditions into account is described below:

Let H(j) be the known value at node number j of the element layout. The coefficient associated with this value in the simplified matrix on the L.H.S. of equation 3.22 is, say, PK (j,j) and the corresponding element of the R.H.S. column matrix, obtained after simplifying the R.H.S. of equation 3.22 is, say, F(j) , which includes the unknown element of [R] also. These values of PK (j,j) and F(j) are replaced by the following new values,

$$PK\ (j,j)_{new} = PK\ (j,j)_{old} * 10^{50}$$

and,

$$F\ (j)_{new} = PK\ (j,j)_{old} * 10^{50} * H\ (j) \quad .$$

Solution of the system of equations 3.22, with the above replacements, would meet the requirements of the given boundary conditions. The multiplier 10^{50} is an arbitrarily chosen large number used to force the given value of H (j) for the nodal point in question to come out as the final solution for that node. It is seen here that the solution procedure does not require [R] to be known.

(iii)A special boundary that has to be treated for the problem under study is the well face. At this boundary, a constant rate of pumping would imply that,

$$H_r \Big|_{r=r_w} = \text{constant, for each length segment.}$$

But, due to non-uniform distribution of discharge along the penetration depth of the well, this constant may not have the same value for all the length segments between adjacent nodes along the well face, Muskat (1946). Therefore, a prerequisite to properly account for the

well-boundary is to estimate the values of this constant applicable to the various nodal points on the well-face. Assuming that the flow at the well-face is purely radial and also assuming that the potential inside the well is the same at every point along the penetration depth, Hantush (1964), an iterative procedure suggested by Muskat (1932) was devised, but it proved to be very time consuming. Further, prior investigations, Hantush (1964) indicated that the gain in accuracy achieved by adopting such an elaborate procedure, is not worth the effort and that in most cases, it is reasonable to assume a uniform distribution of discharge over the penetration depth. Accordingly, for the present investigation, an average value of q_i given by the following equation has been used,

$$q_i = Q_w/2\pi\ r_w \times \text{PENETR}$$

where,

Q_w = well discharge,

PENETR = depth of well penetration,

The subscript i denotes the i^{th} node on the well face.

As explained in Appendix C, the elements of matrix [QK] on the R.H.S. of equation 3.22 may be computed with this known value of q_i for the well-face. It is also known that the unknown [R] contributes nothing on the well-boundary. Thus the R.H.S. of equation 3.22 is completely known for all the nodes along the well face.

3.8 Finite-Element Formulation for the Convective-Dispersion Equation.

Assuming that the velocities u and v, the porosity ϕ, the fluid density ρ and the coefficients of dispersion D^*_{11}, D^*_{22} and D^*_{12} are invariants within an element for a particular time step, the

convective-dispersion equation 3.6 may be expressed in the following form,

$$\frac{1}{r}(r\,D_{rr}\,C_r + r\,D_{rz}\,C_z)_r + (D_{zz}\,C_z + D_{rz}\,C_r)_z - uC_r - vC_z - C_t = 0 \tag{3.23}$$

where,

$$D_{rr} = D^*_{11}\ \frac{\rho}{\rho-\alpha C}$$

$$D_{rz} = D^*_{12}\ \frac{\rho}{\rho-\alpha C}$$

$$D_{zz} = D^*_{22}\ \frac{\rho}{\rho-\alpha C}$$

and D^*_{11} , D^*_{12} and D^*_{22} are as defined in Section 3.2.

The Galerkin Approach. Following the Galerkin approach as discussed in Appendix D, with an arbitrary weighting function W_p and applying the divergence theorem to the weighted residual, as was done for the flow equation, the following equations are obtained,

$$\iint_R [\ (W_p)_r\ (D_{rr}\,C_r + D_{rz}\,C_z) + (W_p)_z\ (D_{zz}\,C_z + D_{rz}\,C_r) + W_p\ (uC_r + vC_z + C_t)\ ]\ r\,dr\,dz = \int_S W_p\ (D_{rr}\,C_r + D_{rz}\,C_z)\ n^1\,dS + \int_S W_p\ (D_{zz}\,C_z + D_{rz}\,C_r)\ n^3\,dS \quad \text{. Where } p=i,j,k\ . \tag{3.24}$$

Using the boundary conditions discussed in Section 3.9, the R.H.S. of equation 3.24 reduces to zero except for the well-face and the boundaries where concentration is invariant with time. For the well-boundary, value of the R.H.S. expression of equation 3.24 is known in terms of the flow rate q and for the boundary where concentration is invariant with time, the expression on the R.H.S. of equation 3.24 may be set equal to some unknown value [R] . It is shown in Section 3.9 that, as

for the flow equation, the value of [R] is not required to be computed for the solution of the resulting system of equations. Substituting these values in equation 3.24 and transforming it to a local coordinate system, the following equations are obtained for the m^{th} element of the layout,

$$\iint_{R^m} [(W_p)_\xi (D_{rr} C_\xi + D_{rz} C_\eta) + (W_p)_\eta (D_{zz} C_\eta + D_{rz} C_\xi) + W_p (uC_\xi + vC_\eta + C_t)] (\bar{r}^m + \xi) \, d\xi \, d\eta = - \int_{S_2^m} W_p \, qC \left(\frac{1}{\phi} - 1 \right) r_w \, d\eta + [R] \quad . \tag{3.25}$$

Defining a continuous shape function [A] as explained in Appendix D, such that,

$$C = [A] \{C\}^m \quad , \tag{3.26}$$

and assuming that this shape function itself is the weighting function, equation 3.25 transforms as follows:

$$\iint_{R^m} \{ ((A_p)_\xi [D_{rr} [A]_\xi + D_{rz} [A]_\eta] + (A_p)_\eta [D_{zz} [A]_\eta + D_{rz} [A]_\xi] + u [A]_\xi A_p + v [A]_\eta A_p) (\bar{r}^m + \xi) \, d\xi \, d\eta \} \{C\}^m + \iint_{R^m} \{ A_p [A] (\bar{r}^m + \xi) \, d\xi \, d\eta \} \{C_t\}^m = - \int_{S_2^m} A_p [A] \, q \left(\frac{1}{\phi} - 1 \right) r_w \{C\}^m \, d\eta + [R] \quad . \tag{3.27}$$

Evaluating the differentials and integrals and writing the resulting system of equations in the symbolic form defined in Appendix D, the

following relationship is obtained for the m^{th} element,

$$[SL]\ \{C\}^m + [PL]\ \{C_t\}^m = -\ [Q]^m + [R]^m \quad . \tag{3.28}$$

Following the usual assembly procedure for combining contributions of all the elements to the various nodes in the layout, the following system of simultaneous equations results,

$$[SK]\ \{C\} + [PK]\ \{C_t\} = -\ [QK] + [R] \quad . \tag{3.29}$$

An important point to be noted here is that the very fact that the convective-dispersion equation (3.23) is not in a self-adjoint form, causes the matrices [SL] and [PL] and, hence, the matrices [SK] and [PK] to be unsymmetric, which is a disadvantage for numerical solutions.

The Rayleigh-Ritz Approach. Since equation 3.6, as such, is not in a self-adjoint form, a reducing factor has to be developed for it. Following Hildebrand (1965), it may be seen (Appendix E) that the required reducing factor is,

$$r \cdot \exp(\beta) \tag{3.30}$$

where,

$$\beta = \frac{v\,D_{rz} - u\,D_{zz}}{D_{zz}\,D_{rr} - D_{rz}^2} \cdot r + \frac{u\,D_{rz} - v\,D_{rr}}{D_{zz}\,D_{rr} - D_{rz}^2} \cdot z$$

$$= -\ \frac{\rho - \alpha C}{\rho} \cdot \frac{ur + vz}{D_L + D_d\,T} \quad .$$

Multiplying equation 3.6 by this reducing factor and for convenience of numerical computation, transforming it in terms of a new variable ψ, such that,

$$\psi = C\ e^{\beta/2} \quad , \tag{3.31}$$

the following equation is obtained,

$$\frac{1}{r}(r\,D_{rr}\,\psi_r)_r + (D_{zz}\,\psi_z)_z + \frac{1}{r}(r\,D_{rz}\,\psi_z)_r + \frac{1}{r}(r\,D_{rz}\,\psi_r)_z =$$

$$\psi_t + (f(r,z) - \frac{u}{2r})\,\psi \quad , \tag{3.32}$$

where,

$$f(r,z) = \frac{u^2\,D_{zz} + v^2\,D_{rr} - 2D_{rz}\,u\,v}{4\,(D_{rr}\,D_{zz} - D_{rz}^2)} \quad .$$

The variational functional for this equation, Hildebrand (1965) reduced to the local coordinate system, with reference to the centroid of the m^{th} element as the origin, as shown in Appendix E is:

$$J = \iint_{R^m} \left[\frac{D_{rr}}{2}(\psi_\xi)^2 + D_{rz}\,\psi_\xi\,\psi_\eta + \frac{D_{zz}}{2}(\psi_\eta)^2 + \psi\left(\frac{u}{2}\psi_\xi + \frac{v}{2}\psi_\eta\right) \right.$$

$$\left. + \frac{\psi^2}{2} f(r,z) + \psi\cdot\psi_t \right] (\xi + \bar{r}^m)\,d\xi\,d\eta + \int_{S_2^m} r_w\,q\left(\frac{1}{\phi} - 1\right)\frac{\psi^2}{2}\,dS \quad , \tag{3.33}$$

where S_2^m refers to the portion of the well-boundary, if any, common with the boundary of the m^{th} element.

The boundary conditions in terms of the new variable ψ are,

(i) $\left.\begin{aligned} D_{rr}\,\psi_r + D_{rz}\,\psi_z + \frac{u\psi}{2} = 0 \\ D_{rz}\,\psi_r + D_{zz}\,\psi_z + \frac{v\psi}{2} = 0 \end{aligned}\right\}$ along natural boundaries,

(ii) $\delta\psi = 0$ along geometric boundaries

(iii) $D_{rr}\,\psi_r + D_{rz}\,\psi_z + \frac{u\psi}{2} - q\left(\frac{1}{\phi} - 1\right)\psi = 0$ along the well face.

It may be shown by equating the first variation of J to zero and by substituting the above boundary conditions in the resulting equation, that equation 3.6 in its transformed form as equation 3.32 is the Euler's equation for the above variational functional. Adopting the

same shape function for ψ, as was assumed for C in the Galerkin approach, so that,

$$\psi = [A] \{\psi\}^m \tag{3.34}$$

and computing the contribution of the m^{th} element to the differentials $J^m_{\psi_p}$ $(p=i,j,k)$, the following equations are obtained,

$$J^m_{\psi_p} = \iint_{R^m} [\, D_{rr} \psi_\xi (\psi_\xi)_{\psi_p} + D_{rz} \{ \psi_\xi (\psi_\eta)_{\psi_p} + \psi_\eta (\psi_\xi)_{\psi_p} \}$$

$$+ D_{zz} \psi_\eta (\psi_\eta)_{\psi_p} + \psi \{ \frac{u}{2} (\psi_\xi)_{\psi_p} + \frac{v}{2} (\psi_\eta)_{\psi_p} \}$$

$$+ (\psi)_{\psi_p} \{ \frac{u}{2} \psi_\xi + \frac{v}{2} \psi_\eta \} + \psi \frac{\rho-\alpha C}{\rho} \cdot \frac{u^2 + v^2}{4(D_L+D_d T)} \cdot (\psi)_{\psi_p}$$

$$+ \psi_t (\psi)_{\psi_p}] (\xi + \bar{r}^m)\, d\xi\, d\eta + \int_{S_2^m} r_w\, q\, (\frac{1}{\phi} - 1)\, \psi\, (\psi)_{\psi_p}\, d\eta = 0 \tag{3.35}$$

where the subscript ψ_p denotes a derivative with respect to ψ_p.

This system, even if the transformation in terms of ψ was not affected, would not be identical to that obtained by the Galerkin method in equation 3.27. Evaluating the differentials and integrals occurring in equation 3.35 will also result in a system of equations of the form,

$$[SL] \{\psi\}^m + [PL] \{\psi_t\}^m + \{Q\}^m = 0 \quad . \tag{3.36}$$

The [SL] and [PL] matrices in this case, though more complicated than those obtained by the Galerkin method, happen to be symmetric (Appendix E). Following the usual assembly procedure, applicable to the finite-element formulation, the follwoing system of simultaneous equations is obtained,

$$[SK] \{\psi\} + [PK] \{\psi_t\} + [QK] = 0 \quad . \tag{3.37}$$

This system is mathematically similar to that obtained in equation 3.29 except for the numerical values of the matrices [SK] and [PK]

and has the additional qualification that the matrices [SK] and [PK] are symmetric. However, the appearance of the variable ψ in place of C , makes it radically different as far as the difficulties in the numerical solution are concerned. The variable ψ involves the exponential of β and thus can not be evaluated by a CDC 6400 computer if the values of β exceed 1483.34 .

As discussed in Chapter IV, this limitation imposes a serious restriction on the practical application of the Rayleigh-Ritz formulation for the solution of the convective-dispersion equation and nullifies the computational advantage that it could have by way of generating symmetric matrices. Therefore, in this investigation the Galerkin method is used.

3.9 Time Domain Formulation of the Convective-Dispersion Equation.

As discussed in Section 3.6, the Galerkin approach may be adopted for the time domain solution of equation 3.29 in preference to the Runge-Kutta and Adams-Moulton schemes. Thus, as before, the equation for the weighted residual becomes,

$$\int_0^{\Delta t} N_1 \left[[PK] \{C_t\} + [SK] \{C\} + [QK] - [R] \right] dt = 0 \qquad (3.38)$$

where,

$$\{C\} = [N] \begin{Bmatrix} \{C\}_0 \\ \{C\}_1 \end{Bmatrix}$$

and

$$[N] = [\, N_0 \quad N_1 \,] = [\, 1 - \frac{t}{\Delta t} \quad \frac{t}{\Delta t} \,] \quad .$$

Evaluating the integrals in 3.38 and collecting terms in $\{C\}_0$ and $\{C\}_1$ separately, gives,

$$\left[\frac{1}{\Delta t} \cdot [PK] + \frac{2}{3} \cdot [SK] \right] \{C\}_1 = - [QK] + [R] + \left[\frac{1}{\Delta t} \cdot [PK] \right.$$

$$\left. - \frac{1}{3} \cdot [SK] \right] \{C\}_0 \quad . \tag{3.39}$$

which is the required recurrence relation to get the values $\{C\}_1$ at time step Δt from known values $\{C\}_0$ at time step 0 in the convective-dispersion equation. An alternative relation obtained by the subdomain method is given in Appendix D.

3.10 Treatment of the Boundary and Initial Conditions for the Convective-Dispersion Equation.

Initial values of C for all the nodal points are specified as initial conditions, say $C_i(r,z)$ etc., As explained in Appendix D, the boundary conditions on the well-face are accounted for in the finite-element formulation through the matrix [QK] of equation 3.39. The unknown [R] contributes nothing for such boundaries and so the R.H.S. of equation 3.39 is fully known. Natural or reflective boundary conditions, specifying $C_n=0$ on impervious boundaries are included in the formulation by setting the R.H.S. terms of equation 3.24 equal to zero. Obviously, both [QK] and [R] will contribute nothing to nodal points on such boundaries. This type of boundary condition applies to the top impermeable layer overlying the confined aquifer and to the vertical stream-line running from the center of the well-bottom down to the lower boundary of the aquifer, across which there is no flow. In this investigation where the well radius r_w is small compared to the element sizes and where the bottom of the well is treated as impermeable, this boundary is approximated to coincide with the vertical running at distance

r_w from the well-center and extending from the well-bottom down to the lower boundary of the aquifer.

Along a section of the aquifer, beyond the radius of influence r_o of the well and at a large depth below the bottom of the well, C remains invariant with time and so may be represented by specified values $C_1(r,z)$, $C_2(r,z)$,...., $C_n(r,z)$ etc.. As explained in section 3.7, such boundary conditions, referred to as geometric boundary conditions, may be accounted for by multiplying the coefficients, say, PK (j,j) of the known values C(j) for the j^{th} node in equation 3.39, by an arbitrarily large number, say, 10^{50} and replacing the original R.H.S. by the value C(j) * PK(j,j) * 10^{50} . This device makes it unnecessary to compute the value of the R.H.S. expression of equation (3.39) which includes the undetermined term [R] for such boundary conditions and at the same time ensures that the value C(j) is maintained on the j^{th} node through successive time steps.

3.11 The Implicit Leap-Frog Technique.

As discussed in the previous sections, given appropriate boundary and initial conditions, the R.H.S. of equation 3.22 is known at time level t_o , in terms of $\{H\}_0$, $\{C\}_0$, $\{\phi\}_0$ and $\{\rho\}_0$, etc.. To start with $\{C_t\}$ may either be specified or taken as zero. The corresponding values at time level $t_o+\Delta t$, are then obtained by solving the system of equations 3.22 by the Gauss-elimination shceme for banded symmetric matrices. This gives the values of $\{H\}_1$ for all the nodes at the next time-step. From these, values of the new pressures $\{P\}_1$ and hence of the new densities $\{\rho\}_1$ and aquifer porosity $\{\phi\}_1$ are computed for all the nodes. Values of elemental velocities u and v at the new time-step are then computed from these known nodal point values $\{H\}_1$,

by applying Darcy's law as follows,

$$u = - \frac{k}{\mu} \cdot H_{\xi}$$

$$v = - \frac{k}{\mu} \cdot H_{\eta}$$

where,

$$H = [A] \{H\}_1 \quad .$$

Therefore,

$$u = - \frac{k}{2\mu A^m} [a_{2i} \quad a_{2j} \quad a_{2k}] \{H\}_1$$

and

$$v = - \frac{k}{2\mu A^m} [a_{3i} \quad a_{3j} \quad a_{3k}] \{H\}_1$$

where the symbols A^m , a_{2i} and a_{3i} , etc. are defined in Appendix C, u , v , k and μ refer to the elemental values and $\{H\}_1$ refer to the already computed nodal point values.

With these values of $\{u\}_1$, $\{v\}_1$ for all the elements and $\{\rho\}_1$ and initially prescribed values of $\{C\}_0$ for all the nodes, the system of equation 3.39 is solved by Gauss-elimination for banded matrices to obtain the values $\{C\}_1$ at the next time-step. With these values of $\{C\}_1$, the density matrix $\{\rho\}_1$ is updated again and values of $\{\rho_t\}$ and $\{C_t\}$ are computed. The values of $\{\rho_t\}$ and $\{C_t\}$ are then used to form a new system of equations, 3.13, which may be solved as before and the above sequence repeated over and over again.

For the purposes of this investigation, however, in order to save computer time without appreciable loss of accuracy, the values of $\{\rho\}$ are updated only once after new values of $\{C\}_1$ are obtained from the solution of the system 3.39 and not twice as indicated above. Further, values of $\{C_t\}$ and $\{\rho_t\}$ are not used to form new systems of equations 3.13 again and again. The changes in $\{C\}$ and $\{\rho\}$ with time being

very small, these simplifications are not expected to introduce appreciable errors. This premise has been corroborated by the resluts discussed in Section 4.4. For cases where these changes are likely to materially affect the results, the above simplifications may be avoided.

CHAPTER IV

DISCUSSION AND APPLICATION OF THE NUMERICAL SIMULATOR

4.1 Description.

The numerical simulator developed in this study is comprised of three computer programs; MESH, FLOW and DISPER. Program MESH is a modified version of an existing one, Thompson[1] (1972) and programs FLOW and DISPER have been written exclusively for this investigation. A description of each of these programs follows:

(a) Program MESH - A listing of this program is given in Appendix H. It incorporates a scheme for generating a suitable element layout for the finite-element solution of any problem. For complex flow regions, the elements have to vary in size depending upon their distances from the well. For this purpose, the flow region is divided into different loops depending upon the nature of the problem, as illustrated in Fig. 4.1. With the input data explained in Appendix G, this program subdivides each loop into a number of quadrilaterals and joins the shorter diagonal of each, as illustrated by representative dashed lines in figure 4.1, to generate a triangular mesh, with specific numbers assigned to all the nodes and elements.

For situations, like the one described in Section 4.3, an alternative element layout with diagonals of the quadrilaterals reversed is also required. To take care of such cases, program MESH has been equipped with an algorithm to produce both the element layouts.

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[1]With the cooperation of Dr. E. G. Thompson, Civil Engineering Department, Colorado State University, Fort Collins.

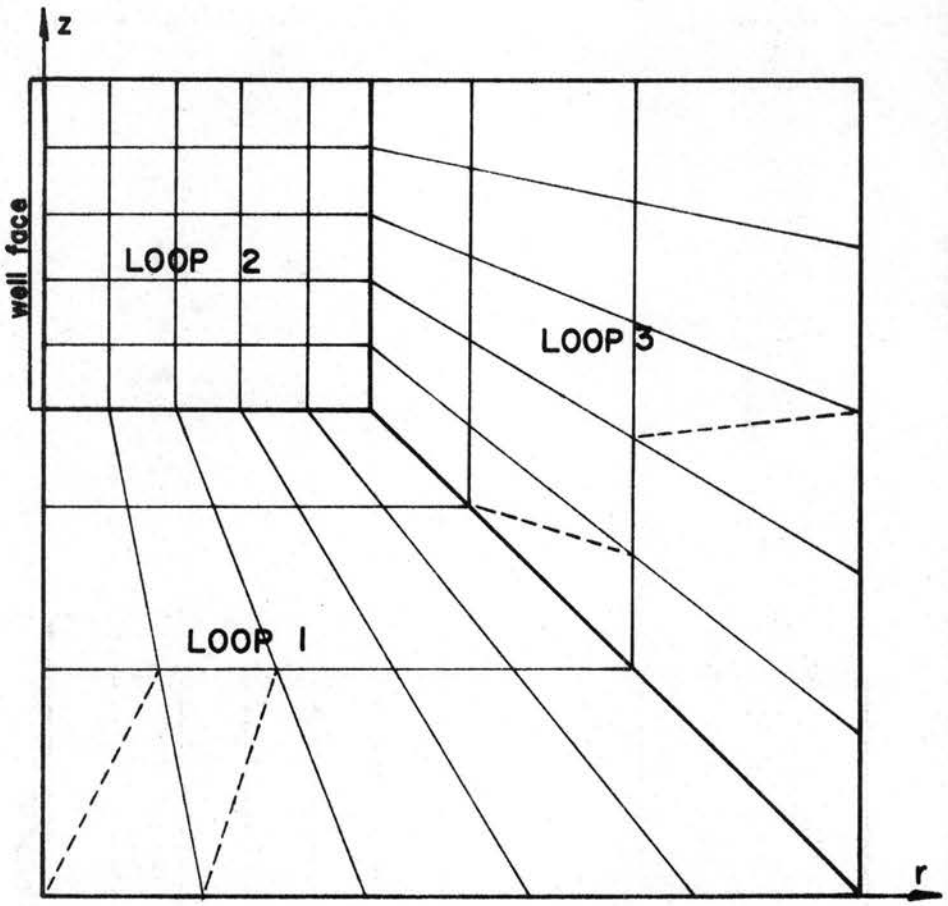

Fig. 4.1 Typical Loop Subdivision

For flow regions with more than two loops, program MESH gives an element layout which has a very large band-width. In order to reduce the band-width, two subroutines, viz. subroutine SETUP and subroutine OPTNUM (Collins, 1973) have been introduced into this version of program MESH. Subroutine SETUP arranges the data generated by repetitive application of the algorithm MESH in the following form:

N	JMEM(N)	MEMJT(N)
Original Node Number	Total number of nodes in the layout to which the Nth node is connected.	Assigned numbers of individual nodes to which the Nth node is connected.

With this information as input, subroutine OPTNUM treats each node as the origin of the new numbering scheme, in turn, so that the number of different renumbering schemes attempted is equal to the total number of nodes in the layout. At each trial, it checks the band-width obtained and finally yields a new numbering scheme that gives the smallest band-width with the initial and modified node numbers identified as follows:

N	JNT(N)
Old Node Number	New Node Number

This information along with the coordinates of each node and the new numbers assigned to the three nodes of each individual element is obtained as a deck of punched cards. This program turns out a microfilm plot of the element layout also.

For simpler flow regions, where the element sizes are not to be varied in both the r and z directions, a simpler version of this program is used, which treats the entire flow domain as one loop and

bypasses the optimization subroutines. Once the orientation of the boundaries is so arranged that node numbering starts in sequence along the side with smaller number of nodes or divisions, this version produces an element layout with a reasonably small band-width.

Program MESH gives the output in x and y coordinates which are read as r and z in programs FLOW and DISPER.

(b) PROGRAM FLOW - As explained in Chapter III, both the Rayleigh-Ritz and Galerkin formulations yield identical matrices for the flow equation. Because these matrices are banded and symmetric, only the upper diagonal elements within the band-width have to be stored, thus reducing the computer storage considerably. Program FLOW solves the flow equation and consists of various subroutines to perform the operations developed in Appendix C. A flow chart describing the various steps involved in this program is given in Appendix F. The subroutines CENTOD, CLOCAL and AREA evaluate respectively the global coordinates of the centroid, local coordinates of the nodal points and the area of each triangular element. Subroutine TEGRAL computes the various volume integrals (reduced to surface integrals due to radial symmetry) involved in the finite-element formulation discussed in Chapter III, using three integration points with Gauss-Radau coefficients for Gauss-quadrature. Subroutine RHOSEL evaluates the average values of the mass-density of the fluid and salt concentration applicable to an element, from given nodal point values. Subroutine FSLPL generates the elemental 3x3 symmetric matrices [FSL] and [FPLE] in terms of the contributions received by each nodal point from the minimization process of the variational functional for the Rayleigh-Ritz formulation and from the weighted-residual process for the Galerkin formulation.

Subroutine FSLSK combines the 3x3 elemental matrices [FSL] and [FPLE] to form the large (NUMNP X IBAND) symmetric matrices [SK] and [PK] and the column vector [QK] representing the contribution of the well, in such a way that all the elemental contributions to any node common to two or more elements are added up and the diagonal elements (i,i) of the original (NUMNP X NUMNP) matrices are stored as the first elements (i,1) of each row in the rearranged (NUMNP X IBAND) matrices. The symbol NUMNP used herein signifies the total number of nodal points and IBAND stands for the band-width for symmetric matrices as defined in Chapter III. Subroutine FSKPSI multiplies the rearranged matrix SK(NUMNP, IBAND) with a column vector PSI(NUMNP) . Subroutine GAUSS solves the above system of NUMNP simultaneous equations by Gauss-elimination in such a way that only the upper diagonal elements are used in the process. This yields values of H for all the nodes at the new time level, from where nodal point pressures are readily obtained and elemental volocities u and v are computed by applying Darcy's law as explained in Chapter III.

(c) PROGRAM DISPER - Unlike the flow equation, the convective-dispersion equation, as such, is not in a self-adjoint form, mainly because of the presence of first derivative and mixed partial terms. Therefore, the Rayleigh-Ritz and Galerkin formulations do not yield identical system of matrices. Whereas the former yields symmetric matrices, the latter leads to a system of unsymmetric matrices. For reasons discussed later, the Galerkin formulation has been adopted for this study, although programs were written and run for both. The program DISPER seeks to solve the convective-dispersion equation by the Galerkin-weighted-residual technique. A flow chart for this program is

given in Appendix F. This program consists of various subroutines accomplishing the operations described in Appendix D. Subroutines CENTOD, CLOCAL, AREA and TEGRAL are exactly the same as for FLOW. Subroutine ELVEL computes the average elemental velocities from known values of nodal point pressures. Subroutine SLPL generates the 3x3 nonsymmetric elemental matrices [SL] and [PL] pertaining to each element.

Subroutine SLSK combines the matrices [SL] and [PL] to form the large (NUMNP X IBAND) unsymmetric matrices [SK] and [PK] and the column vector [QK] having NUMNP elements to account for the contribution of the well. The symbol IBAND here refers to the band-width for unsymmetric matrices as defined in Chapter III. The elements of matrices [SK] and [PK] are so arranged that element (i,j) of the original (NUMNP X NUMNP) banded unsymmetric matrices becomes element [i, (j-1 + (IBAND + 1)/2)] of the contracted (NUMNP X IBAND) matrices. Subroutine SKPSI is a modified version of its counterpart in program FLOW, and multiplies the (NUMNP X IBAND) matrix [SK] with a column vector PSI(NUMNP). Subroutine BSOLVE solves this system of NUMNP simultaneous equations by Gauss-elimination with row interchanges. This yields nodal point values for the concentration at the new time step.

4.2 Leap-Frog Technique and Program FFLOW.

As indicated in Chapter III, the two programs, FLOW and DISPER, work in tandem in the leap-frog technique and so have been merged together into a composite program, FFLOW. A flow chart for the leap-frog technique is given in Appendix F. With given initial values of ρ , ϕ and P for each nodal point, next time values of P are computed in program FLOW (incorporated within FFLOW). Knowing new time P values, the elemental velocities u and v are computed. With these values of u and v

and given initial values of nodal point concentrations, next time values of the latter are computed in program DISPER (incorporated within FFLOW). At this stage, with the current values of nodal point P and C , values of nodal point density and porosity are updated. With these new values of ρ , ϕ and P as input, program FLOW operates again to yield the next time values of P and thus the process of iteration is continued until the required time period is completed. A listing of the combined program FFLOW is attached in Appendix H.

4.3 Tests for the Performance of the Numerical Simulator.

In the absence of pertinent experimental or field data, the results of the combined program FFLOW can not be verified. However, programs FLOW and DISPER have been tested separately by comparison with known exact and approximate solutions for simplified radial flow cases. A description of these tests is given below.

(a) Program FLOW - In order to test the validity and accuracy of the finite element formulation for the flow equation, the well known case of unsteady radial flow towards a well in a confined aquifer was run as a test with the following data:

Radius of well - r_w = 0.5 ft.

Well discharge - Q = 1.0 ft^3/sec.

Depth of well penetration = PENETR = 100 ft.

Aquifer thickness = B = 100 ft.

Assumed radius of influence = r_e = 950.5 ft..

The very nature of the finite-element formulation, specially for cases where the aquifer depth is divided into very few divisions, tends to yield unequal values of H for various nodal points along the same vertical in the vicinity of the well, even for cases of pure radial

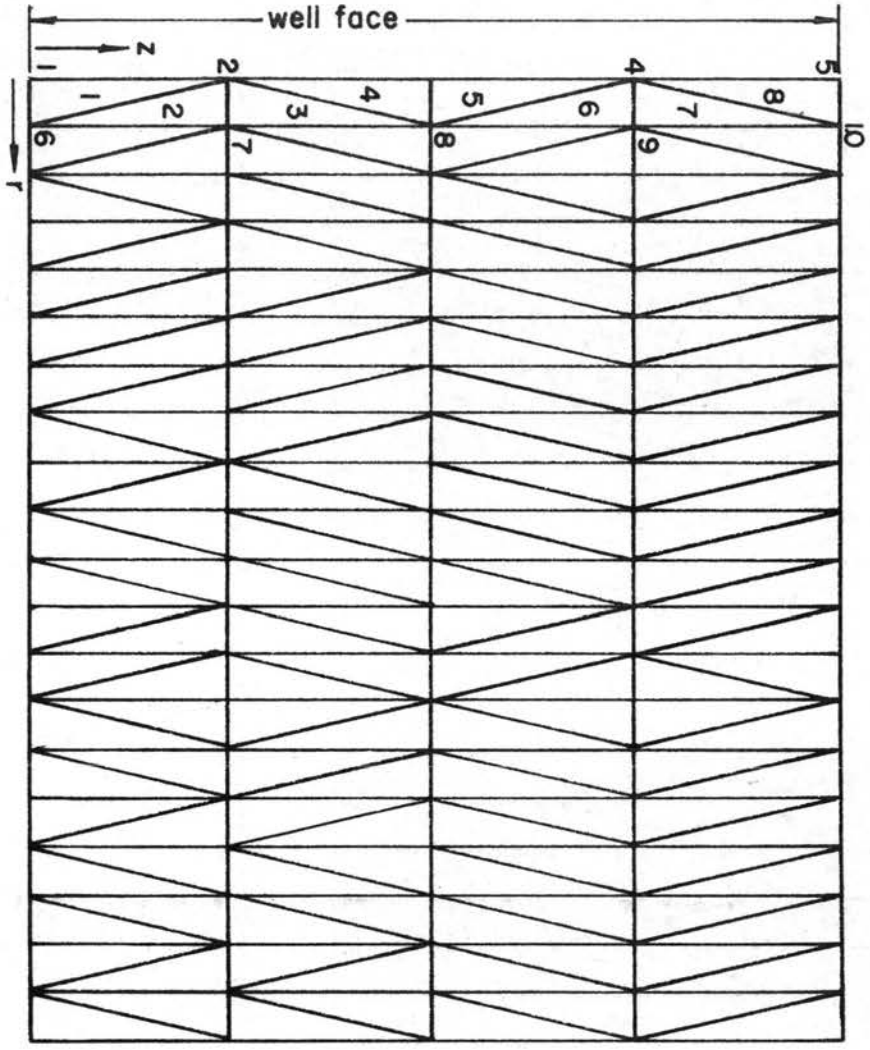

Fig. 4.2a Typical Element-Layout

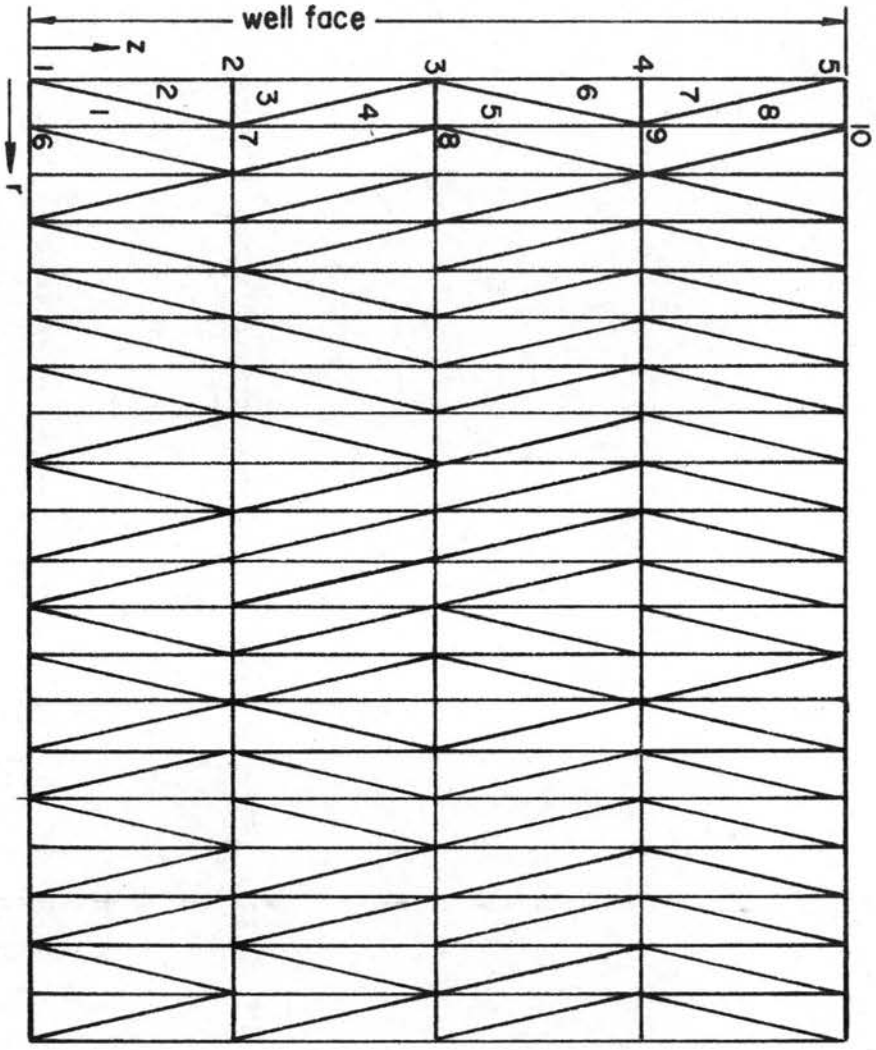

Fig. 4.2b Alternative Element Layout with Diagonals Reversed

flow. This occurs because of different weightages assumed by different nodes in a triangular layout due to their geometric placement. To resolve this, the [SK] and [PK] matrices are formed twice for each iteration, once for the original element layout as given by the program MESH and next for the alternative layout with the diagonals of quadrilaterals forming individual elements, reversed as shown in Figs. 4.2a and 4.2b. The averages of these two sets of [SK] and [PK] matrices are then taken as the final [SK] and [PK] matrices. This results in the allocation of equal weightage to all the nodal points on a vertical and thus yields equal values of H for such nodal points for purely radial flow.

The element layout was obtained from program MESH with the following data:

XMIN = 0.0 ft. (Minimum value of the x-coordinate).

XMAX = 100 ft. (Maximum value of the x-coordinate).

YMIN = 0.5 ft. (Minimum value of the y-coordinate).

YMAX = 950.5 ft. (Maximum value of the y-coordinate).

NDIVX = 2 (Number of divisions along the x-axis).

NDIVY = 95 (Number of divisions along the y-axis).

The output of the MESH program gave,

NUMNP = 288 (Number of nodal points).

NUMEL = 380 (Number of elements).

IBAND = 5 (Band-width for symmetric matrices).

Analytical solution for this case is available as follows, Walton (1970):

$$s = \frac{Q}{4\pi T} \quad W(u) \qquad (4.1)$$

where,

s = drawn down in feet at time t and distance r from well center.

$T = kB$ = Aquifer transmissibility in $ft^2/sec.$

k = Hydraulic conductivity in ft/sec.

$u = \frac{Sr^2}{4Tt}$.

S = Storage coefficient of the aquifer = $\gamma B(\phi\beta + C_F)$.

γ = Unit weight of the fluid in lbs/ft^3.

B = Aquifer thickness in feet.

t = Time at which drawdown s occurs at distance r from the well center.

$W(u) = \int_u^\infty \frac{e^{-u}}{u} du$ = Well function.

ϕ = Porosity, taken as 0.5 for this test.

β = Fluid compressibility in sq. ft./lb.

C_F = Aquifer compressibility in sq. ft./lb.

The results of the numerical and analytical solutions are shown in Fig. 4.3. It is seen that the results are in excellent agreement. The minor differences of about 4 to 10% in the drawdown at the well face may be attributed to two factors, viz. larger size of elements and smaller radius of influence used. The analytical solution assumes an infinite radius of influence against 950.5 ft. used in the numerical solution. Also accuracy demands that smaller size elements should be used in the vicinity of the well, whereas equal size elements have been used in the mesh layout for the above numerical solution. With smaller size of elements provided near the well and with larger radius of influence, the solution will become more and more accurate even at the well face.

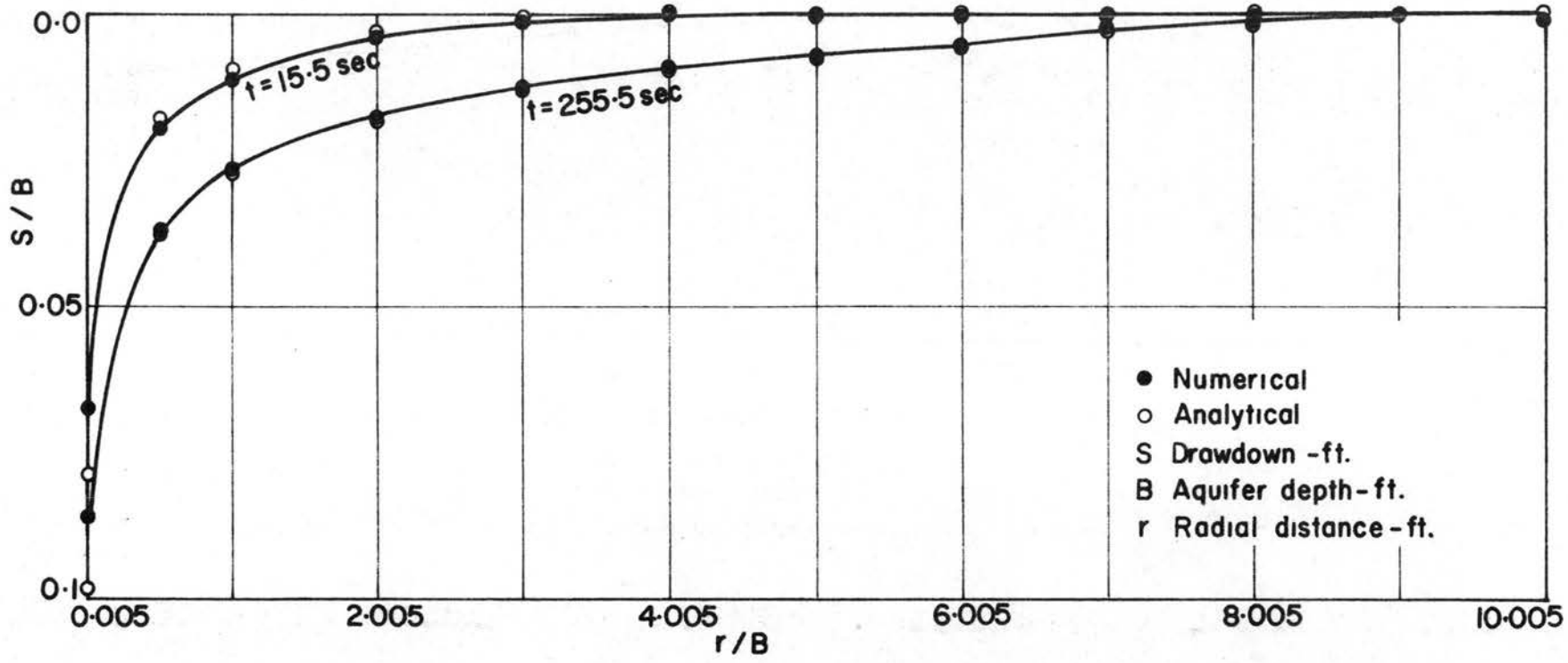

Fig. 4.3 Analytical and Numerical Solutions of Flow Equation

Since program DISPER constitutes different subroutines for matrix multiplication and Gauss-elimination, it was run on the same set of data as was used for program FLOW with a view to verify the validity of the formulation for unsymmetric matrices involved in program DISPER. The input data was modified so that the dispersion equation becomes identical to the flow equation, treating concentration C as synonimous with the variable H . The two runs of program FLOW and program DISPER on identical data yielded identical results up to 8 significant figures for all the 8 iterations for which comparison was made, thus establishing the equivalence, accuracy and correctness of the two programs. Representative values for the 7^{th} iteration at time 2.5 seconds are reproduced in Table 4.1 for comparison.

TABLE 4.1
COMPARISON OF PROGRAM FLOW AND DISPER

Radial Distance ft.	Values of H (lbs/ft^2)	
r	PROGRAM FLOW	PROGRAM DISPER
0.5	7935.96014469	7935.960001
50.5	8075.27685378	8075.276814
100.5	8113.05940422	8113.059394
200.5	8124.93396647	8124.933966
300.5	8124.99956215	8124.999562

(b) PROGRAM DISPER - In order to test the accuracy of the program and formulation for the convective-dispersion equation, program DISPER was run for a dispersion-dominated transport until steady state. The numerical solution was assumed to have reached steady state when the change in concentration at any point between two time steps was less than 0.00001 . For such a case, steady state solution may be analytically

obtained. Setting,

$$D_{rz} = D_{zz} = 0 \quad , \quad \text{and} \quad v=0$$

the convective-dispersion equation, 3.6, reduces to,

$$C_r = \frac{D_o}{A} C_{rr} \tag{4.2}$$

where,

$$A = \frac{Q}{2\pi \text{ X PENETR X } \phi}$$

$$D_o = a_I \cdot A$$

and the subscript rr denotes second derivative with respect to r .

For the boundary conditions,

$C = C_o$ at $r = r_w$ and,

$C = 0$ at $r = r_o$,

equation 4.2 may be solved to yield,

$$\frac{C}{C_o} = \left[\exp\left(\frac{Ar}{D_o}\right) - \exp\left(\frac{Ar_o}{D_o}\right)\right] / \left[\exp\left(\frac{Ar_w}{D_o}\right) - \exp\left(\frac{Ar_o}{D_o}\right)\right] \tag{4.3}$$

Results of the analytical solution of equation 4.3 have been compared with the numerical solution run until steady state, in Fig. 4.4. For this case, steady state was reached after 830 seconds. The excellent agreement of the two solutions demonstrates the accuracy and convergence of the dispersion part of program DISPER.

To test the validity of the formulation for the convective-dispersion equation for a situation where the contributions of both dispersion and convection are equally dominant, program DISPER was run for the case of purely radial flow in a confined isotropic aquifer, for which an approximate analytical solution is available, Hoopes and Harleman (1965); Shamir and Harleman (1966). For such a case, assuming that

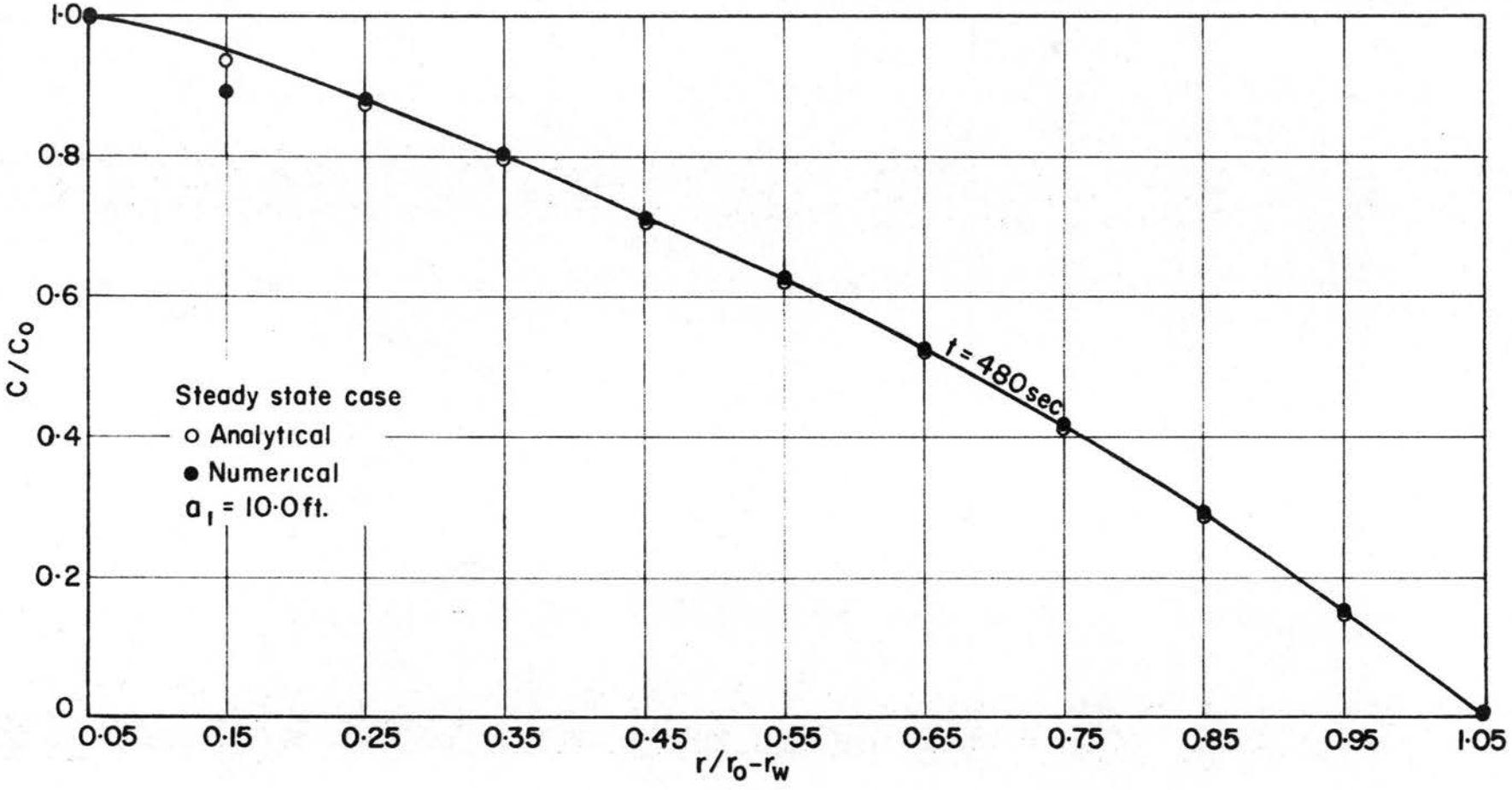

Fig. 4.4 Steady-State Solutions of Convective-Dispersion Equation

$$D_T = 0 \quad , \quad D_d = 0 \quad , \quad v = 0 \quad \text{and} \quad \rho = \text{constant},$$

the convective dispersion equation (3.6) reduces to the following form,

$$(D_L\, C_r)_r + \left(\frac{D_L}{r} - u \right) C_r = C_t \quad . \tag{4.4}$$

Recognizing that,

$$D_L = a_I\, u = a_I \cdot \frac{Q}{2\pi x \text{PENETR} x \phi x r}$$

$$= a_I \frac{A}{r} = \frac{D_o}{r} \quad , \tag{4.5}$$

equation 4.4 may be written as,

$$C_t + \frac{A}{r} C_r = \frac{D_o}{r} C_{rr} \quad . \tag{4.6}$$

An approximate analytical solution to equation 4.6 has been given by Raimondi et al. (1959) for the case when a tracer is injected at r=0 for a finite time period. The same has been modified by Hoopes and Harleman (1965) for the case of continuous injection of a tracer of constant concentration, C_o at r=0 . Their solution is as follows:

$$\frac{C}{C_o} = \frac{1}{2} \text{erfc} \left[\frac{r^2/2 - At}{\sqrt{\frac{4}{3} a_I\, r^3}} \right] \quad . \tag{4.7}$$

It may be seen that this solution satisfies the two boundary conditions,

$$C\ (r=0\ ,\ t>0) = C_o \qquad \text{and}$$

$$C\ (r=\infty\ ,\ t \geq 0) = 0 \qquad ;$$

but does not satisfy the initial condition,

$$C\ (r\ ,\ t=0) = 0 \quad .$$

In obtaining this solution, it has been assumed that,

$$C_t = 0 \quad \text{at} \quad t = 0 \quad ,$$

which is not true in the immediate vicinity of the source. Thus the approximate solution of equation 4.7 holds only for points away from the source.

The element layout for this case was also obtained from program MESH, with the following input data:

XMIN = 0.0 ft. , XMAX = 1.0 ft. ,

YMIN = 0.5 ft. , YMAX = 10.5 ft. ,

NDIVX = 4 , NDIVY = 20 .

The output of program MESH gave,

NUMNP = 105 , NUMEL = 160 , and IBAND = 7 .

Program DISPER was run with,

$a_I = 1.0$ ft.

$Q = .25$ ft^3/sec.

$\phi = 0.5$.

Results of the numerical and approximate analytical solutions are presented in Fig. 4.5 for two representative time periods. The agreement between the two solutions is reasonable for points away from the source for which the approximate analytical solution is applicable. Because of the assumption made to arrive at equation 4.7, the solution does not hold for steady state cases also. However, for a steady state case, equation 4.6 reduces to equation 4.2 and so the solution given by equation 4.3 holds. Comparison of this exact solution for steady state with the numerical solution has also been shown in Fig. 4.5. The steady state was reached after 2330 seconds. The two solutions are in excellent agreement.

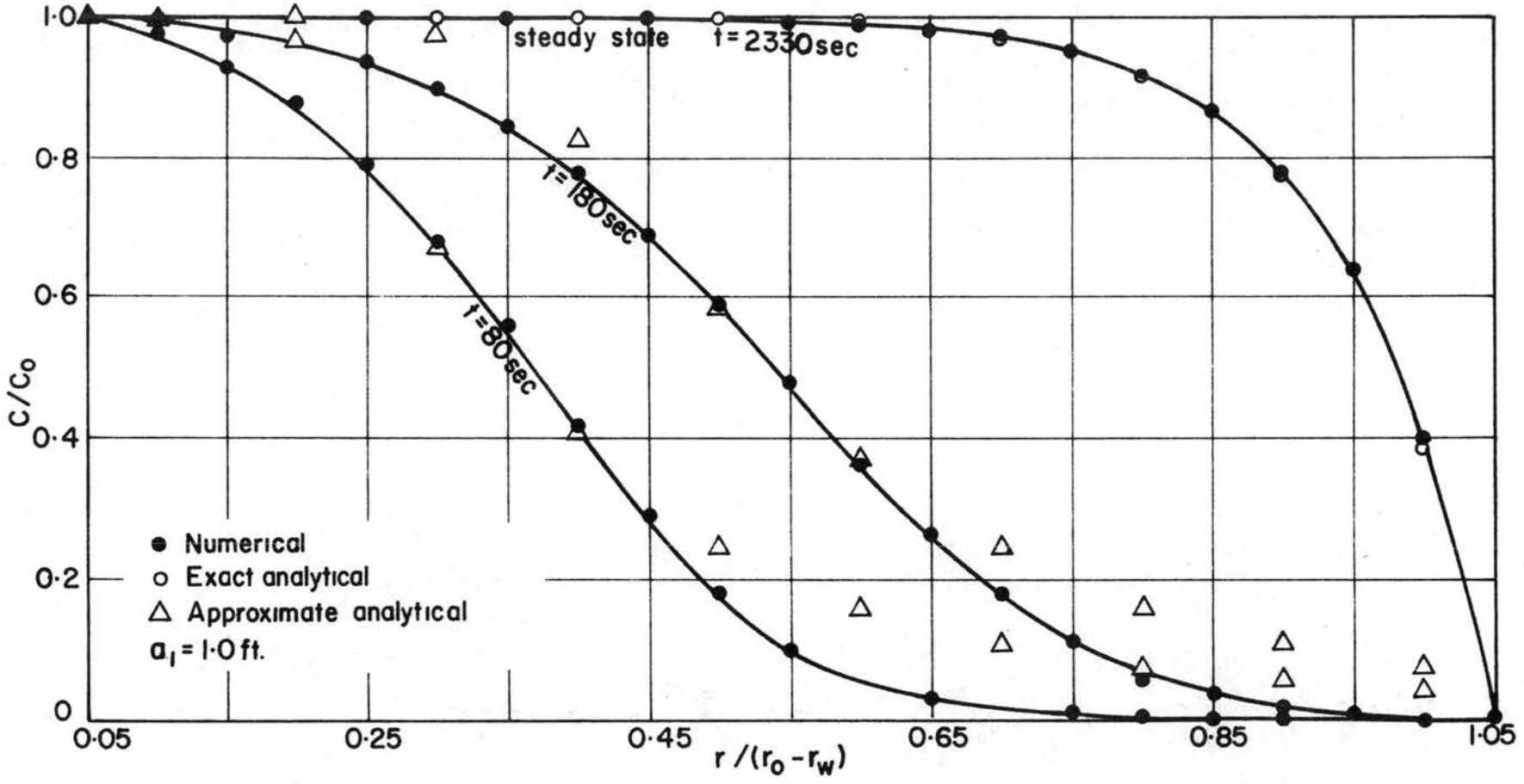

Fig. 4.5 Analytical and Numerical Solutions of Convective-Dispersion Equation, a_I = 1.0 foot

Program DISPER was run for a convection dominant transport also, using the same data as was used for the previous two runs except for the value of a_I which was taken as 0.1 ft. for this case. Results of the numerical and analytical solutions are depicted in Fig. 4.6 both for the transient and steady-state cases. The agreement between the two solutions is reasonable.

It is noted that the agreement improves as the distance from the source increases. This is due to the fact that the approximate solution holds only for points away from the source. In this case, steady-state reached after 730 seconds, whereafter no marked change was observed in the concenteration distribution. As for the provious case, the numerical solution for steady-state has been compared with the exact solution and not with the approximate solution, which holds only in the transient state.

A comparative picture of the three types of transports with different geometric dispersivities, discussed above, has been presented in Fig. 4.7, where the propagation of concentration with time has been plotted for all the three cases for one and the same point in the flow-domain. Both the numerical and approximate analytical values have been indicated on the three plots.

For all the three cases, the numerical solution is in reasonable agreement with the approximate solution in the transient zone and with the exact solution after steady-state is reached. These plots corroborate the well known effect of dispersion to flatten out the break-through curve. The effect gets more and more pronounced with increasing values of the geometric dispersivity of the soil.

The various tests discussed in this section prove the validity and accuracy of the numerical finite-element models developed in this study.

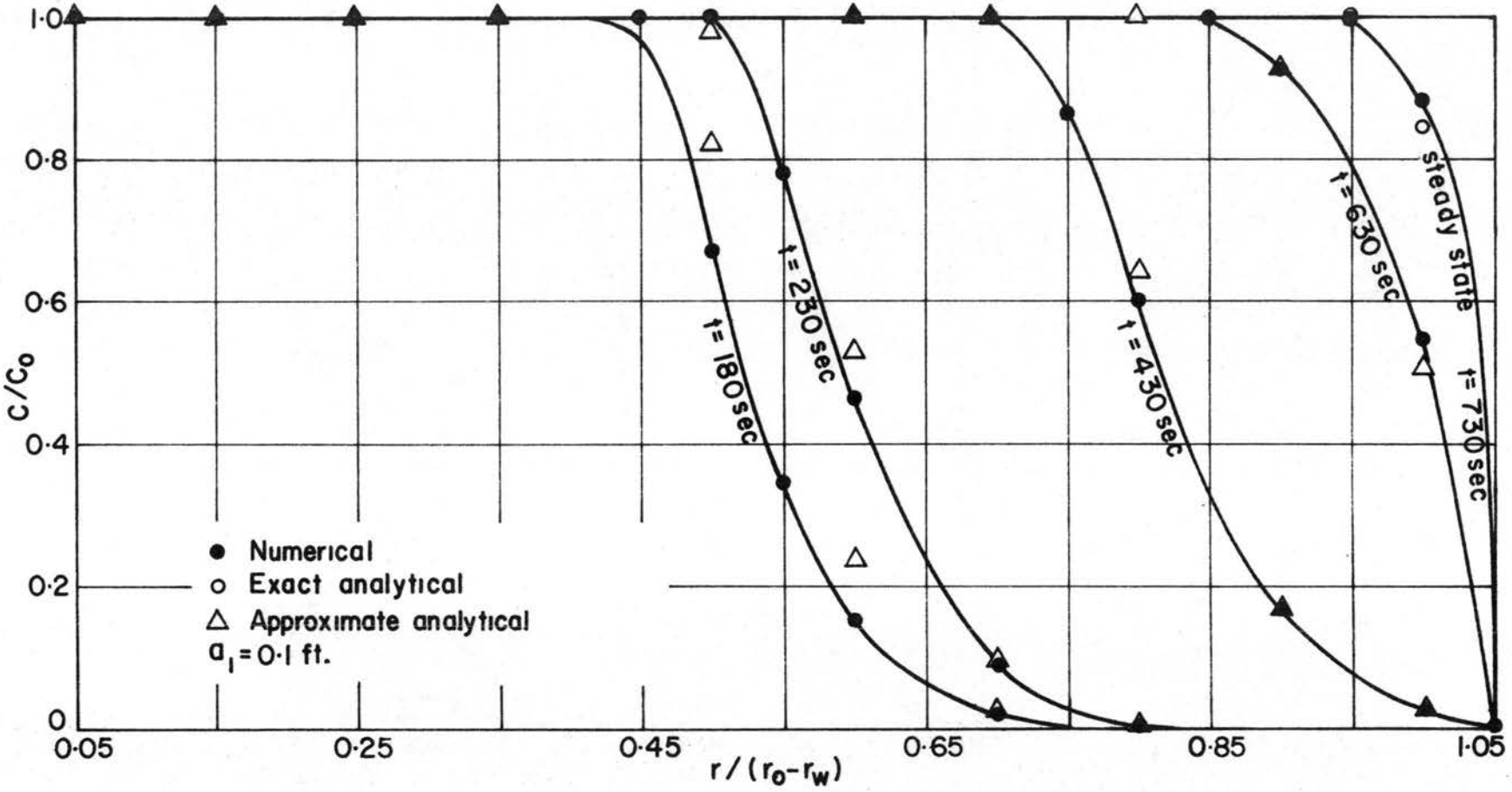

Fig. 4.6 Analytical and Numerical Solutions of Convective-Dispersion Equation, a_I = 0.1 foot

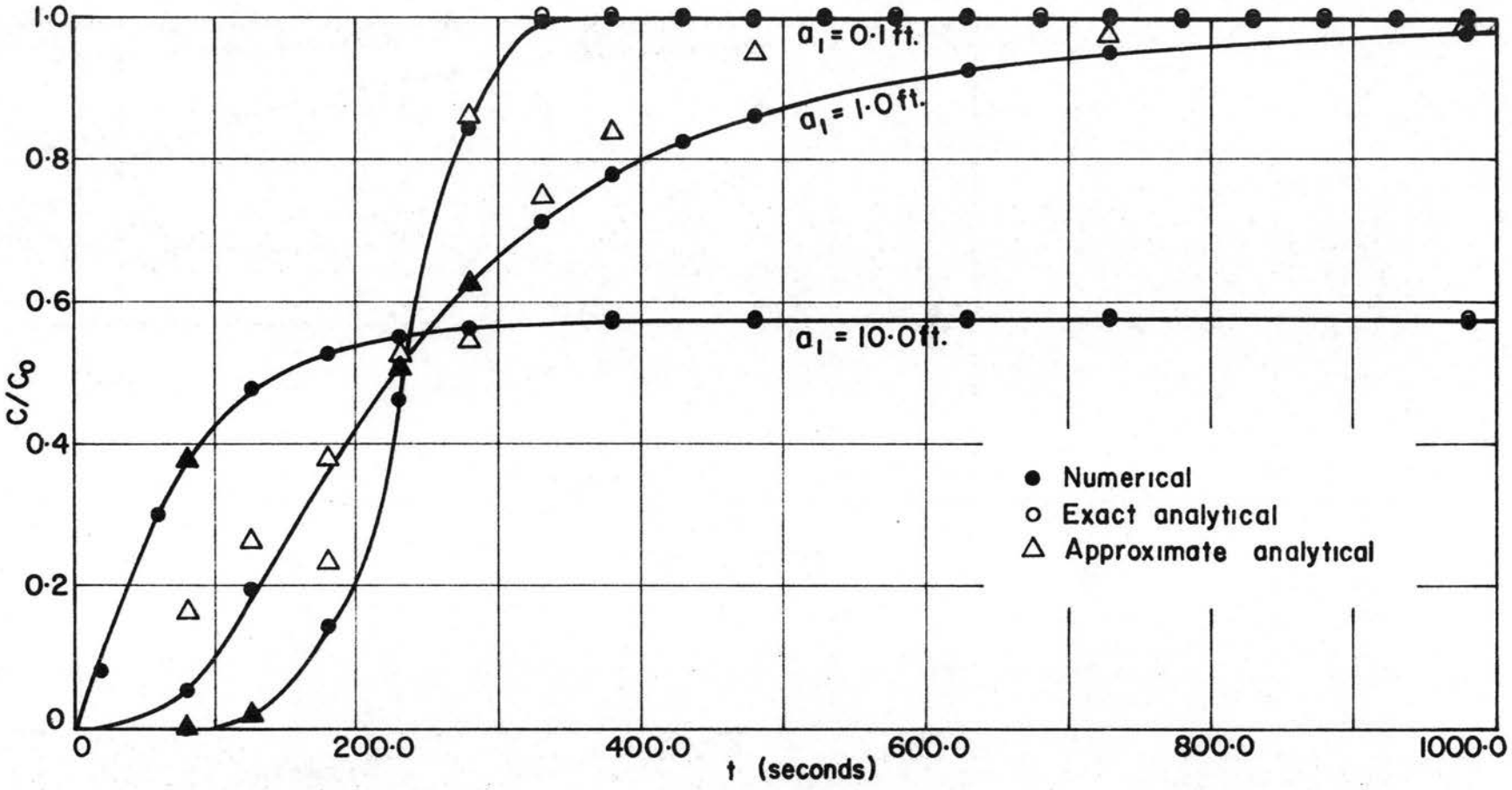

Fig. 4.7 Propagation of Concentration with Different Geometric Dispersivities

4.4 Application of the Simulator to Field Problems.

In order to demonstrate the capability of the simulator to solve field problems, two hypothetical cases were run, one for a confined aquifer having a salt-water reservoir as its outer boundary and being pumped by a fully penetrating well, and the other for a very deep aquifer containing fresh water underlain by very deep belts of salt-water and being pumped by a partially penetrating well. Element layouts for both these cases were generated by using program MESH. The data used for these cases are tabulated on the following page.

The values 780.5 and 510.5 feet used for the radius of influence of the well in these cases are smaller than those expected for a field situation. This was done to save computer time and storage. Taking advantage of the dynamics of the problem, the convective-dispersion equation was solved only once with time step Δt for every ten solutions of the flow equation with time step $\Delta t/10$. Even with these expedients, the concentration propagated only 160 feet over a period of 2.29×10^8 seconds (7.26 years) for the fully penetrating well case. This took 300 iterations and 2000 seconds of C. P. time on the CSU CDC 6400 computer. The compilation time was only 14.685 seconds. For these iterations, the time step was successively increased from 0.1 second at the first iteration to 1,000,000 seconds at the 80^{th} iteration, whereafter, it was maintained at this value through the 300^{th} iteration.

For the partially penetrating well case, it took 2.2×10^7 seconds (255 days) for the concentration to propagate 90 feet involving 320 iterations and 3600 seconds of C. P. time. The compilation time was only 14.714 seconds. As in the previous case, the time step was successively increased from 0.1 second at the first iteration to 100,000

TABLE 4.2. DATA FOR HYPOTHETICAL PROBLEMS

DATA	Fully penetrating well with a salt water reservoir as the outer boundary.	Partially penetrating well with a salt water reservoir as the lower boundary.
(a) FOR PROGRAM MESH:		
XMIN	0.5 ft.	0.5 ft.
XMAX	780.5 ft.	510.5 ft.
YMIN	0.0 ft.	0.0 ft.
YMAX	100.0 ft.	300.0 ft.
(b) FOR PROGRAM FFLOW:		
NUMNP	200	198
NUMEL	312	340
Q	2.0 $ft^3/sec.$	4.0 $ft^3/sec.$
r_w	0.5 ft.	0.5 ft.
PENETR	100.0 ft.	120.0 ft.
ϕ_o	0.5	0.5
α	0.74	0.74
β	2.3×10^{-8} $ft^2/lb.$	$2.3\times10^{-8} ft^2/lb.$
C_F	0.6×10^{-8} $ft^2/lb.$	$0.6\times10^{-8} ft^2/lb.$
μ	2.4×10^{-5} $lb.sec./ft^2$	$2.4\times10^{-5} lb.sec./ft^2$
ρ	2.0 $slugs/ft^3$	2.0 $slugs/ft^3$
a_I	0.1 ft.	1.0 ft.
a_{II}	0.0 ft.	0.1 ft.
D_d	0.0 $ft^2/sec.$	0.0001 $ft^2/sec.$
H	8125.0 ft.lbs.; $r\geq780.5, t\geq0$ 8125.0 ft.lbs.; $r<780.5, t=0$	54,000.0 ft.lbs.; $r\geq510.5, t\geq0$ 54,000.0 ft.lbs.; $z\leq0, t\geq0$ 54,000.0 ft.lbs.; $r<510.5, z>0, t=0$
C/C_o	1.0 ; $r\geq780.5, t\geq0$ 0.0 ; $r<780.5, t=0$	1.0 ; $z\leq0, t\geq0$ 0.0 ; $z>0, t=0$

seconds at the 110^{th} iteration, whereafter, it was maintained at that value through the 320^{th} iteration.

The propagation of concentration with time at two representative locations in the flow field for both these cases, has been shown in Figs. 4.8 and 4.9. Although these plots lack verification with experimental models or with actual field data, they do demonstrate the capability of the simulator to handle such field problems. The qualitative trends depicted by these runs indicate that for a normal size well, the computer time required for the concentration to appear in the well discharge might be of the order of 10,000 seconds or so and the actual time of travel might be in the range of a few years depending upon the aquifer properties.

In both these cases, the values of H tend to become almost steady after a certain time level as may be seen from the values tabulated below:

TABLE 4.3. H-VALUES AT THE WELL FACE AFTER PROLONGED PUMPING

Time (seconds)	Full Penetration Case	Time (seconds)	Partial Penetration Case
1.2×10^{8}	7168.4994	7.2×10^{6}	53973.1828
1.3×10^{8}	7168.5129	8.2×10^{6}	53973.1830
1.4×10^{8}	7168.5276	9.2×10^{6}	53973.1833
1.5×10^{8}	7168.5436	10.2×10^{6}	53973.1837

After prolonged pumping beyond the transient state, the only variables that change and affect the values of H are the fluid density and aquifer elasticity. Stationarity of the H values in the above table indicates that the effects of variable fluid density and aquifer elasticity on the transport process are very small.

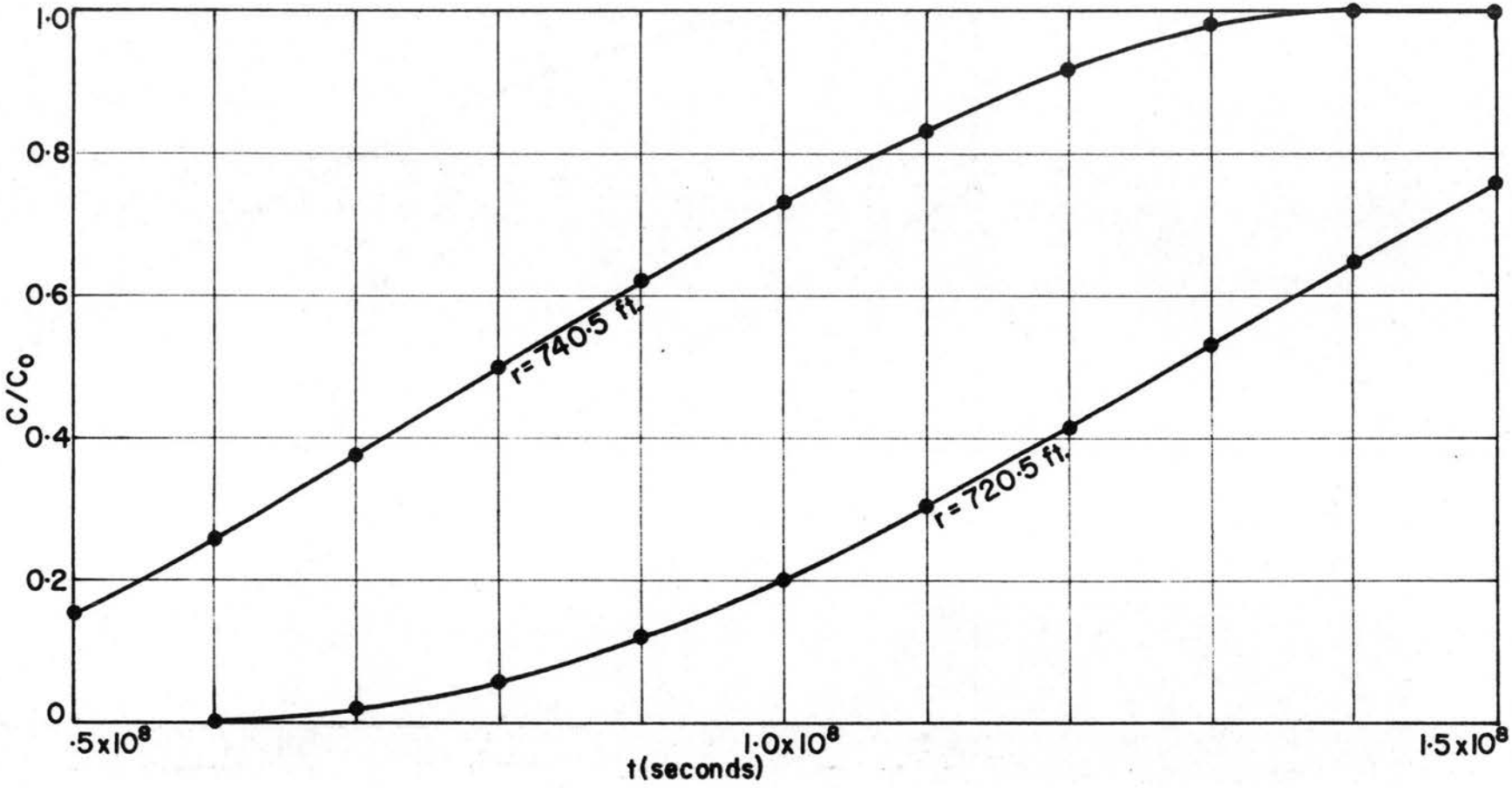

Fig. 4.8 Propagation of Concentration for a Fully Penetrating Well

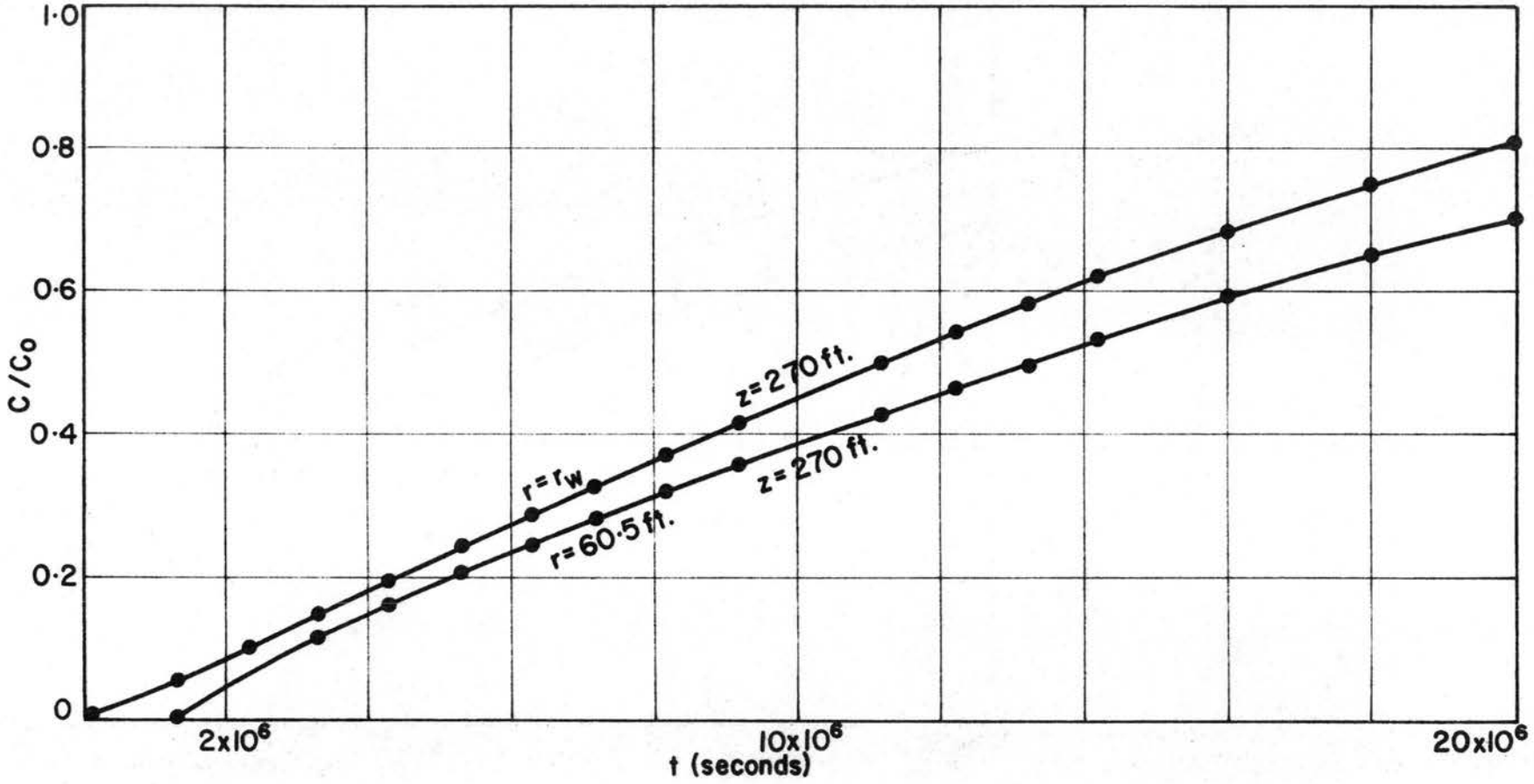

Fig. 4.9 Propagation of Concentration for a Partially Penetrating Well

4.5 Galerkin and Rayleigh-Ritz Simulators.

As already stated the Rayleigh-Ritz formulation has a significant advantage over the Galerkin in so far as it, almost always, yields symmetric matrices. The Galerkin formulation, on the other hand, leads to unsymmetric matrices except for self-adjoint systems. Therefore, this study was initially started with the Rayleigh-Ritz formulation in view, but the exponential transformation function β , so essential for the Rayleigh-Ritz formulation of the convective-dispersion equation, 3.16, which is not in a self-adjoint form (Appendix E), makes it almost impossible to follow the method on a computer. The β transform function and the transformed variable ψ are defined as (Appendix E),

$$\beta = - \frac{ur + vz}{D_d T + D_L} \cdot \frac{\rho - \alpha C}{\rho}$$

and

$$\psi = C \cdot e^{\beta/2} \quad .$$

For large radii of influence or for deep aquifers, the values of β for the exterior nodes or elements may easily exceed the limit of 1483.34 for a CDC 6400 computer and so it may not be possible to evaluate β at nodes or elements far away from the origin, for normal values of the coefficient of hydrodynamic dispersion. For transports that are highly convection dominant,such a difficulty arises even for nodes or elements moderately away from the origin. Since, in most cases of salt-water dispersion and diffusion in saturated soils, the contribution of hydrodynamic dispersion is small and the transport is convection-dominant, the method, though mathematically elegant, has a serious limitation for practical problems in geohydrology.

In pursuance of this method for the solution of cases pertinent to this investigation, an attempt was made to extend the limits up to which this formulation could be handled by the CDC 6400 machine, by dividing the previous time values of ψ at all the nodes by a constant sufficiently large in value to bring the largest ψ value within the computer range without letting the smallest ψ value go below the lowest limit of the computer, viz. $e^{-741.67}$. Obviously, even this device could work only within twice the range of the original limits and therefore, the method still remained far from general. Besides, the vary nature of the β transform function, yields very widely different ψ values for nodes near and far from the origin, even though the corresponding concentration values may be more or less equal. Thus, the same order of truncation error in the Gauss-elimination at such nodes, manifests itself into largely vitiated results. These difficulties with the Rayleigh-Ritz formulation appear to be insurmountable at this stage. Therefore, this method was abandoned in favour of the Galerkin.

For practical well-flow problems, the regions to be simulated are of the order of 1000 feet or so in radial length and aquifer depths vary from 200 feet to 1000 feet. Following the mesh pattern discussed in section 4.1(a), with reasonable element sizes, the band-width for symmetric matrices for such regions might easily be as high as 16 even after band-width reduction; which for unsymmetric matrices obtained in the Galerkin formulation rises to 33 . With such a large band-width, a moderate element layout even with 150 nodes, would yield [SK] and [PK] matrices of size (150x33) . For larger number of nodes, the band-width will further rise and consequently, the storage requirement for the [SK] , [PK] and their auxiliary matrices becomes prohibitive.

Besides, the diagonal inversion technique for developing an alternative element layout indicated in Section 4.3(a), if adopted, would produce such a large band-width that the storage requirement will become prohibitive. However, this plausibly insurmountable impediment of the Galerkin process may be overcome by a judicious use of auxiliary tape storage. This, in no way, is too great a disadvantage, in view of the versatility of the formulation for handling cases of any order of convection or dispersion dominated transports.

4.6 Stability and Convergence.

By definition unstable methods are those in which growth of individual round off errors, inherent in the inexact arithmetical operations performed by the computer, causes a significant and unwarranted error in the computed solution. In such schemes, a decrease in step size may reduce the inherent error of the method but may increase round off errors by a much greater amount. A particular solution is said to be stable if the propagated errors are bounded. On the other hand, convergence is the property of a numerical solution to tend to the exact solution with finer and finer discretising functions. For the numerical simulator developed in this investigation, stability and convergence have to be studied from the following view-points:

(i) Solution in the space domain.

(ii) Solution in the time domain.

(iii) Integration scheme.

(iv) Data input.

The finite-element solution of the problem in the space-domain results in an implicit scheme, yielding a set of simultaneous equations to be solved by Gauss-elimination and so is inherently stable. However,

sometimes difficulties might arise with non-homogeneous problems, described by matrices which are not diagonally dominant for some particular element layout. For such cases the problem can be alleviated by changing the node numbering pattern by trial and error until non-singular diagonally dominant matrices with positive diagonal entries are obtained. As the properties of the [SK] and [PK] matrices generated for the space-domain solution are dependent upon the geometry and size of individual elements, it is important to be judicious in choosing a suitable mesh with almost equilateral triangles. With regard to the convergence, it has been observed that the finer the mesh the more accurate is the solution.

TABLE 4.4. H-VALUES AFTER 55.5 SECONDS OF PUMPING

r	Analytical Solution	Numerical Solution	
		380 Element Mesh	240 Element Mesh
.5	7558.60	7641.49	7795.97
50.5	7951.43	7945.48	7946.93
100.5	8012.18	8004.06	8004.24
200.5	8070.60	8059.60	8059.99
300.5	8082.46	8087.86	8088.12
400.5	8108.07	8104.11	8104.29
500.5	8124.88	8113.61	8113.76
950.5	8125.00	8125.00	8124.59

The above values demonstrate the convergence of the numerical solution to the analytical solution at the well face, as the mesh is made finer. Values at points away from the well are not appreciably affected.

For the time domain solution, the Galerkin or the Sub-domain method, which ever is employed, results in an implicit formulation and so is potentially stable. Yet, if the choice of time increment is large, the

accumulation of round off errors may render the solution unacceptably inaccurate. This type of divergence from the true solution is sometimes termed as induced instability. However, if higher order interpolation functions are used for the time dependence, greater stability of solution is obtained and larger time increments may be used. For the problem at hand, since both the flow and convective-dispersion equations are solved in sequence and since the former is a faster process than the latter, the flow equation is solved for a much smaller time interval than the convective-dispersion equation. For large initial time intervals, the flow equation tends to exhibit oscillations, which may be avoided by gradually increasing the time step as shown in the following table.

TABLE 4.5. H-VALUES AT WELL FACE WITH DIFFERENT VALUES OF DT.

DT(sec)	TIME(sec)	H	DT(sec)	TIME(sec)	H
5.0	5.0	7505.77	0.1	1.0	7639.59*
	10.0	7948.51	1.0	10.1	7434.39*
	15.0	7507.50	10.0	110.1	7227.94*
	20.0	7889.13	100.0	1110.1	7168.44*
	25.0	7508.71			

* These values are the same as were used in Fig. 4.3.

Time intervals ranging from 0.1 to 100,000 seconds in successive iterations have been found sufficiently accurate and stable. The solution tends to converge to exact values with smaller and smaller time intervals.

Coming to the integration scheme, convergence of the finite-element process occurs if the integrals evaluated in subroutine TEGRAL are sufficiently accurate. Whereas, it is not possible to quantify the term 'sufficiently accurate', it may be stated qualitatively that if fewer

elements are used to represent the flow region, then larger number of integrating points are desirable in the Gauss-quadrature scheme, to ensure reasonably fast convergence. For the cases analyzed in this investigation, results obtained with three integrating points per triangle matched with those obtained with exact integrations up to eight decimal places. Representative values are tabulated below.

TABLE 4.6. CONCENTRATION DISTRIBUTION AFTER 146.0 SECONDS

r ft.	Gauss Quadrature	Exact Integration
0.5	.99191130	.99191130
1.5	.99418559	.99418559
2.5	.98790338	.98790338
3.5	1.00063250	1.00063250

Trial runs with different data input displayed no convergence or stability porblems. Unlike the method of Guymon and Nalluswami, the method has worked well with values of the geometric dispersivity of the aquifer ranging from 0.1 to 10.0 and can admit even smaller or higher values without blowing up and so there appears to be no need to define a convergence parameter like the one specified by Guymon (1970b) for the Rayleigh-Ritz formulation in cartesian coordinates for a uniform flow system.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

5.1 Summary.

The complex problem of salt-water movement induced by pumping from an aquifer is not amenable to exact mathematical analysis. Numerical techniques developed by past investigators to analyze miscible displacement problems in general, have been limited to uniform rectilinear flow of homogeneous fluids. In this investigation, the flow equation governing the movement of a non-homogeneous, compressible fluid in an isotropic, elastic saturated aquifer, in response to well pumping has been developed in a general system of coordinates. The convective-dispersion equation describing the movement of an inert tracer in the above non-uniform flow field, under isothermal conditions, has also been derived. In this derivation, tensorial nature of dispersion and contribution of molecular diffusion have been taken into account, which were not included in earlier investigations.

A new version of the Galerkin-finite-element approach has been developed for both the space and time domain solutions of the flow equation in cylindrical coordinates. Using the flow parameters so obtained, velocity distribution in the non-uniform flow field is computed. This velocity distribution is used to develop the space and time domain Galerkin formulation for the convective-dispersion equation. To account for fluid non-homogeneity and aquifer compressibility, the variables fluid-density and aquifer porosity are updated at each time-step before passing on to the next iteration. These aspects were not considered in previous investigations.

Boundary conditions, which are of common occurrence in field problems, have been incorporated in the formulation. Natural or reflective boundary conditions are not required to be explicitly entered into the program. Geometric boundary conditions may be introduced as data and taken care of by simple devices provided in the program. Contribution of the well as a sink is evaluated separately and is distributed over all the points lying along the well face. Treatment of the well face boundary conditions has not been attempted by previous investigators.

An efficient scheme has been developed for generating a mesh layout which could represent the complex flow pattern around partially penetrating wells. This scheme incorporates an algorithm to minimize the band-width of the matrices obtained in the finite-element formulation.

Finally, a numerical simulator has been developed incorporating the scheme for automatic mesh generation and the Galerkin-finite-element formulations for the flow and convective-dispersion equations. The validity of this simulator has been tested for the flow and convective-dispersion parts separately. Results of the flow equation match the solution of Theis equation for confined flow cases and those of the convective-dispersion equation compare well with the approximate solution given by Shamir and Harleman. Applicability of the simulator to practical problems has been demonstrated by analyzing two hypothetical field situations. The results of the hypothetical problems could not be verified in the absence of field or experimental data.

5.2 Evaluation and Practical Applications of the Simulator.

The simulator could be used for steady, unsteady, uniform or non-uniform flow and miscible displacement problems, with constant or

variable fluid density and with constant or variable aquifer porosity. Even variable viscosity may be taken care of with minor modifications. A wide range of values for the coefficients of dispersion, from zero to several hundreds or more, may be used without encountering computational problems such as those experienced by Guymon and Nalluswami.

The schemes used for the space and time domain solutions are implicit and inherently stable. For large initial time steps, the flow equation solution scheme tends to exhibit oscillations. This may be overcome by selecting a small initial time step followed by gradually increasing step size at successive iterations without experiencing instability or oscillations. A remarkable advantage of the simulator over the finite-difference model is that no approximation is involved in obtaining pressure and concentration values on the well-face.

The simulator is very versatile and can be applied to the following field situations with or without modifications:

(i) Movement of salt-water from a low lying bed of saline water towards a partially penetrating well. This type of situation exists in the Indus Basin, Pakistan.

(ii) Salt-water intrusion into a coastal aquifer due to pumping by a fully or partially penetrating well. The zigzag pattern of the constant head and constant concentration ocean boundary may easily be represented by triangular elements laid in a zigzag fashion.

(iii) Dispersion of liquid industrial or domestic wastes through recharge pits in an aquifer, induced by natural gradients or by discharging wells near by.

(iv) Movement of contaminants in an open channel and back flow of salt-water in an estuary due to tidal waves in an ocean. This type of

problems do not require the formulation in cylindrical polar coordinates and the well-face boundary conditions.

(v) Cooling of large cylindrical containers by cooler fluid injection through centrally located cylindrical sources. This problem is similar to the recharging well cases discussed in Chapter IV, except that the concentration is replaced by temperature.

5.3 Limitations and Suggestions for Future Work.

Although the simulator developed in this study is quite versatile, yet the various assumptions made at different stages, do warrant further research and study to evaluate the effect and validity of such simplifications. Some of the aspects not covered in this investigation, which require attention of future investigators are:

(i) The interpolation functions used for polynomial representation of the variables C and H, both in the space and time domains are linear. For more accuracy and stability even with coarser element layout and larger time-step size, it would be worthwhile to investigate how the results are affected, if parabolic or higher order interpolation functions with isoparametric elements are used. This investigation is especially important in view of the fact that for actual field aquifers, the number of elements required for reasonably accurate results with linear interpolation functions, has to be very large, requiring huge (sometimes prohibitive) amounts of computer storage. Also, the time required for the concentration to advance from the farthest or deepest point in the aquifer to the well, is so large, that with smaller time increments, inevitable for the linear interpolation function, the number of iterations to be performed becomes extremely large.

(ii) Although the mesh pattern generated can be optimized to yield a minimum band-width, if either the shorter or the larger of the two diagonals of every quadrilateral is joined to form triangular elements, nevertheless, sometimes, for finer meshes, even this minimized band-width turns out to be too large for unsymmetric matrices, causing formidable storage problems. To cope with such situations, the Gauss-elimination scheme needs to be reorganized in such a way that the moment the elements of [SK] and [PK] matrices corresponding to a particular node are generated, their elimination process is completed simultaneously and the result is stored on a tape. In this way, it may be possible to save a considerable amount of storage.

(iii)A thorough investigation needs to be carried out to develop criteria for arriving at an optimum time increment for a non-oscillatory behavior of program FLOW without unduly increasing the number of time steps required to reach a certain time level.

(vi) The simulator developed applies rigorously to a confined aquifer case. Possible extension and modification of the technique for solving unconfined flow problems needs to be investigated.

(v) In the development of flow and convective-dispersion equations in this study, the aquifer has been assumed to be fully saturated and the flow-field has been treated to be under isothermal state. It appears interesting to extend the work for unsaturated soils where thermal-gradient-actuated-flow is significant and needs to be taken into account.

(vi) A more complicated, though desirable, extension of the work is to study the effect of anisotropy and non-homogeneity of the aquifer on the movement of a tracer, induced by well-pumping. This will involve

consideration of the coefficient of dispersion as a fourth rank tensor with all the 36 components and the tortuosity and permeability to be treated as tensors and not scalars as assumed in the present investigation.

(vii)In this investigation, presence of only an inert tracer has been considered. The study needs to be extended to chemically active and radio-active tracers. This will require retention and quantification of the terms for chemical or radio-active reactions in the flow and convective-dispersion equations, which have been tacitly omitted in Appendices A and B.

(viii)In this investigation, it has been assumed that the discharge is uniformly distributed over the penetration depth. It is desirable to examine the difference in the results if the same potential is assumed to exist at every point inside the well, with non-uniform discharge distribution.

(ix) The simulator needs to be applied to and tested on an actual field situation for which observed concentration values at different spacings from the well for different periods of time and at different rates of pumping are available. Aquifer properties like permeability, porosity, tortuosity, geometric dispersivities and formation compressibility along with the coefficient of molecular diffusion, fluid compressibility, viscosity and density must be known with reasonable accuracy from reliable experimentation.

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LIST OF SYMBOLS

Some of the symbols have multiple definitions. Relevant definitions are given wherever such symbols are used in the text.

$[A]$	Reducing factor, shape function	
A_1, A_2	Functions of v^2 and the properties of the fluid, medium and tracer	
A_i, A_j, A_k	Components of the vector $[A]$	
A^I_{ijk}	A third rank tensor	
$A^{II}_{ji\ell k}$	A fourth rank tensor	
A^m, A	Area of the m^{th} triangular element	L^2
$a_{ij\ell m}$	Geometric dispersivity of the porous medium, a fourth rank tensor	L^2T^{-1}
a_I	Longitudinal constant of dispersion or longitudinal dispersivity of the medium	L^2T^{-1}
a_{II}	Lateral constant of dispersion or lateral dispersivity of the medium	L^2T^{-1}
B^I_{jk}	Tortuosity tensor	
C or c	Tracer concentration	ML^{-3}
C_F	Formation compressibility	$M^{-1}LT^2$
C_o	Reference value of concentration	ML^{-3}
C_p	Tracer concentration in the production or consumption fluid	ML^{-3}
D_d	Coefficient of molecular diffusion	L^2T^{-1}
D_{ij}	Dispersion coefficient (A second rank tensor)	L^2T^{-1}
D^*_{ij}	Coefficient of hydrodynamic dispersion	L^2T^{-1}
D_L	Longitudinal dispersion coefficient	L^2T^{-1}

D_{rr}	$D^*_{11} \cdot \rho/(\rho-\alpha c)$	L^2T^{-1}
D_{rz}	$D^*_{12} \cdot \rho/(\rho-\alpha c)$	L^2T^{-1}
D_T	Lateral dispersion coefficient	L^2T^{-1}
D_{zz}	$D^*_{22} \cdot \rho/(\rho-\alpha c)$	L^2T^{-1}
D^*_{11}	$D_dT + D_T + (D_L - D_T)\, v_r^2/v^2$	L^2T^{-1}
D^*_{12}	$(D_L - D_T)\ v_r\, v_z/v^2$	L^2T^{-1}
D^*_{21}	D^*_{12}	L^2T^{-1}
D^*_{22}	$D_dT + D_T + (D_L - D_T)\, v_z^2/v^2$	L^2T^{-1}
$D_{\alpha\beta}$	Average molecular diffusivity	L^2T^{-1}
d	Particle size of the medium	L
E	Variable representing the product $\rho_o\phi_o(\beta + C_F)$	$L^{-2}T^2$
F	Variable representing the product $\alpha\phi_o$	
F_{ci}	Convective component of the mass flux in i direction	$ML^{-2}T^{-1}$
F_d	Diffusive component of the mass flux	$ML^{-2}T^{-1}$
F_{ti}	Total mass flux of the tracer in i direction	$ML^{-2}T^{-1}$
g	Accelaration due to gravity or absolute value of the determinant of g_{ij}	LT^{-2}
g_{ij}	Diagonal matrix of the squares of scale factors for coordinate transformation or fundamental tensor of the Reimanian space (covariant components)	
g^{jk}	A second rank symmetric contravariant tensor, conjugate or reciprocal of g_{ij}	
h_i	Scale factors for coordinate transformation	
H	Piezometric head in energy units i.e., flow parameter $(P + \rho gz)$	$ML^{-1}T^{-2}$

J_i	Macroscopic tracer mass flux in i direction	$ML^{-2}T^{-1}$
J	Variational functional	
k	Permeability	L^2
k_r	Relative permeability to fluid	
k_i	Absolute permeability in i direction	L^2
L	Linear boundary over which line integral is taken	
ℓ	Characteristic length	
m_i	Mass of species i in the reference volume	M
[N]	Shape function	
n	Unit outward normal	
p	Pressure	$ML^{-1}T^{-2}$
P_o	Reference pressure	$ML^{-1}T^{-2}$
P_e	Peclet Number	
Q	Production or consumption term	L^3T^{-1}
Q_w	Well discharge	L^3T^{-1}
q	Seepage velocity along the stream line or Darcy velocity or flow velocity	LT^{-1}
q_i	Volume flux through the face perpendicular to i or Darcy velocity in i direction	LT^{-1}
R	Region of space, An arbitrary coefficient	L^2
R_m^n	Rate of production or consumption of constituent n in the m^{th} reaction	$ML^{-3}T^{-1}$
[R]	Symbolic representation for unknown terms in an expression	
r	Radial coordinates - Number of sources or sinks in the system	L
$\bar{r}^m$	r - coordinate of the centroid of m^{th} element	L

S	Saturation or	
	variable representing the expression $\frac{\rho k}{\mu}$	T
T	Scalar tortuosity	
T_{ij}	Tortuosity tensor	L^{-2}
t	Time	T
u	Component of seepage velocity in x or i or r	
	direction	LT^{-1}
$\overline{V}$, V	Average Darcy velocity	LT^{-1}
v	Average seepage velocity or	LT^{-1}
	seepage velocity component in z direction	LT^{-1}
v_i	Seepage velocity component in i direction	LT^{-1}
v_o	Fluctuation of seepage velocity about the mean	LT^{-1}
W_p	Weighting function	
x, x_i, or x^i	x - coordinate	L
y	Variable representing the sum EP + FC or	ML^{-3}
	y - coordinate	L
z	Elevation of the volume element above an arbitrary	
	datum which is normal to the direction of gravity	
	z - coordinate	L
$\bar{z}^m$	z - coordinate of the centroid of the m^{th} element	L
α	Proportionality factor relating concentration with	
	density	
β	Fluid Compressibility or	$M^{-1}LT^2$
	argument of the exponential in the reducing	
	factor or	
	experimentally determined coefficient	
γ	Unit weight of water	$ML^{-2}T^{-2}$

δ	Small variation	
δ_{ij}	Kronecker delta	
η	Ordinate in the transformed (local) coordinate system	L
λ	Arbitrary constant used for tensor transformation	
μ	Dynamic viscosity or arbitrary constant used for tensor transformation	$ML^{-1}T^{-1}$
ν	Kinematic viscosity	L^2T^{-1}
ξ	Abscissa in the transformed (local) coordinate system	L
ρ	Mass density of the fluid	ML^{-3}
ρ_o	Reference mass density of the fluid	ML^{-3}
ρ_p	Mass density of the fluid in the source or sink term	ML^{-3}
τ	Dimensionless variable representing time	
ϕ	Porosity	
ϕ_o	Reference porosity	
ψ	Stream function or transformed value of the concentration C or a concentration parameter	ML^{-3}

APPENDIX A

DERIVATION OF THE FLOW EQUATION

The flow equation is obtained by combining the pertinent equation of motion with the continuity equation.

CONTINUITY EQUATION:

Considering mass-balance for a mixture of fluids of several chemical constituents over a control volume D, with $\vec{n}$ as the unit outward normal to the boundary ∂D of D,

$$\int_{\partial D} \rho^k \phi S\, v_i\, n_i\, d\sigma = -\left[\int_D \rho^k \phi s\, dv\right]_t + \sum_{m=1}^{s} \int_D R_m^k\, dv - \int_D w^k{}_\delta\, dv \qquad \text{(A-1)}$$

where,

ρ^k = Mass of constituent k per unit volume of the mixture - (ML^{-3})

ϕ = Porosity of the medium

S = Saturation of the medium

v_i = Seepage velocity component in i direction - (LT^{-1})

$d\sigma$ = An element of the boundary of D - (L^2)

dv = An element of the volume of D - (L^3)

R_m^k = Rate of production or consumption of the constituent k in the m^{th} reaction - $(ML^{-3}T^{-1})$

s = Total number of reactions taking place

$w^k{}_\delta$ = Cumulative equivalent of all the sources or sinks present in the control volume.

$$w^k{}_\delta = \sum_{j=i}^{r} Q^k(x_{1j}, x_{2j}, x_{3j})\, \rho_p^k\, \delta(x_1 - x_{1j})\, \delta(x_2 - x_{2j})\, \delta(x_3 - x_{3j})$$

$- (ML^{-3}T^{-1})$

Q^k = Source or sink effect pertaining to constituent k - (L^3T^{-1})

δ = Dirac delta function

r = Number of sources or sinks of constituent k

x_1, x_2, x_3 = General space coordinates

$x_{1_j}, x_{2_j}, x_{3_j}$ = Space coordinates of the location of the j^{th} source or sink.

ρ_p^k = Mass concentration of constituent k in the source or sink fluid - (L^3T^{-1})

and the subscript t denotes derivative with respect to time. Using divergence theorem, equation A-1 yields,

$$\int_D \{ (\rho^k \phi S v_i)_{,i} + (\rho^k \phi S)_t - \sum_{m=1}^{s} R_m^k + Q^k \rho_p^k d_{\frac{1}{p}} \} dv = 0 \qquad \text{(A-2)}$$

where the comma denotes covariant derivative. $d_{\frac{1}{p}}$ is a variable continuous on D, so that $d_{\frac{1}{p}} \to \delta$ as $\frac{1}{p} \to \infty$.

Since the integrand of A-2 is continuous and the region D is arbitrary,

$$(\rho^k \phi S v_i)_{,i} + (\rho^k \phi S)_t - \sum_{m=1}^{s} R_m^k + Q^k \rho_p^k d_{\frac{1}{p}} = 0 \quad \forall \ \frac{1}{p} \ . \qquad \text{(A-3)}$$

Therefore, as $\frac{1}{p} \to \infty$,

$$(\rho^k \phi S v_i)_{,i} + (\rho^k \phi S)_t - \sum_{m=1}^{s} R_m^k + Q^k \rho_p^k \delta = 0 \ . \qquad \text{(A-4)}$$

Assuming that,

(i) There are no reactions going on in the system,

(ii) There is only one constituent in the mixture so that the superscript k may be dropped,

(iii) There are no sources or sinks in the system,

equation A-4 reduces to,

$$\text{div}(\rho q) = - (\rho \phi S)_t \tag{A-5}$$

where,

q = Macroscopic flux vector with component q_i in i direction

$q_i = v_i \, \phi S \quad - (LT^{-1})$.

But in tensor notation,

$$\text{div}\,(\rho q) = \nabla_i \, (\rho q)^i$$

$$= \rho \nabla_i q^i + q^i \nabla_i \rho$$

$$= \frac{\rho}{\sqrt{g}} \left(\sqrt{g} \cdot q_i \, g^{ij} \right)_{,j} + g^{ij} q_j \, \rho_{,i}$$

$$= \frac{\rho}{\sqrt{g}} \left(\sqrt{g} \, \frac{q_i}{h_i^2} \right)_{,i} + \frac{q_i}{h_i^2} \, \rho_{,i} \tag{A-6}$$

where, g is the absolute value of the determinant of the metric tensor g_{ij} and h_i $(i=1,2,3)$ are the scale factors of coordinate transormation.

Substituting equation A-6 into A-5, collceting derivatives of ρ on one side, transferring terms and dividing out by ρ ,

$$(\phi S)_t + \frac{1}{\sqrt{g}} \left(\sqrt{g} \, \frac{q_i}{h_i^2} \right)_{,i} = - \frac{\phi S}{\rho} \rho_t - \frac{q_i}{h_i^2} \, \rho_{,i} \tag{A-7}$$

which is the required continuity equation.

EQUATION OF MOTION:

Assuming that,

(i) Darcy's law holds for the flow situation under consideration,

(ii) Axes of the coordinate system coincide with the axes of the permeability tensor,

(iii) The system is under isothermal state,

(iv) There is no contribution to flow due to thermodynamic gradients, due to any electrical charge carried by wet soil particles or due to adsorptive force gradients,

the appropriate equation of motion (Darcy's law) may be written as follows:

$$q_i = v_i \phi S = - \frac{k_i k_r}{\mu} \left(\frac{1}{h_i} P_{x_i} + \frac{\rho g}{h_i} z_{x_i} \right) \qquad \text{(A-8)}$$

where, h_i = Scale factor of coordinate transformation

k_i = Absolute permeability in i direction at S=1 - (L^2)

k_r = Relative permeability at saturation S - (L^2)

μ = Dynamic viscosity of the fluid - $(ML^{-1}T^{-1})$

P = Fluid pressure - $(ML^{-1}T^{-2})$

g = Gravitational acceleration - (LT^{-2})

z = Elevation of the volume element above an arbitrary datum, which is normal to the direction of gravity - (L) .

It may further be assumed that the fluid density ρ , pressure P and concentration C are inter-related by a first order equation of state,

$$\rho = \rho_o + \rho_o \beta \, (P - P_o) + \frac{\alpha}{\bar{v}_o} \sum_{i=1}^{n} (m_i - m_o) \qquad \text{(A-9)}$$

where, n = Number of constituents in the mixture

β = Compressibility of the fluid - $(M^{-1}LT^{-2})$

P_o = Reference pressure - $(ML^{-1}T^{-2})$

$\rho_o = \sum_{i=1}^{n} \rho_{io}$

ρ_{io} = Mass of constituent i per unit volume of solution at the reference pressure - (ML^{-3})

m_i = Mass of constituent i in the reference volume $\bar{v}_o$ at the prevailing pressure - (M)

m_{io} = Mass of constituent i in the reference volume $\bar{v}_o$ at the reference pressure - (M)

$\bar{v}_o$ = Reference volume of the fluid mixture (L^3)

α = Proportionality factor

ρ = Mass density of the mixture at pressure P and solute concentration $m_i/\bar{v}_o$ - (ML^{-3}) .

For solutes having only one constituent, equation A-9 reduces to,

$$\rho = \rho_o + \rho_o\beta\,(P - P_o) + \alpha\,(C - C_o) \qquad \text{(A-10)}$$

where, C and C_o are the concentrations (mass of solute per unit volume of solution) at the prevailing state and at the reference state respectively.

Assuming that there is no change in volume upon mixing of fluids of different ionic concentrations and that the factors α and β are independent of pressure and fluid composition,

$$\left.\begin{aligned} \rho_{x_i} &= \beta\rho_o P_{x_i} + \alpha C_{x_i} \\ \rho_t &= \beta\rho_o P_t + \alpha C_t \end{aligned}\right] \qquad \text{(A-11)}$$

where the subscripts x_i and t denote derivatives with respect to them.

FLOW EQUATION:

The flow equation may now be obtained by assuming that k_i and k_r are independent of pressure, temperature and concentration and substituting the equation of motion (A-8) into the continuity equation (A-7),

$$(\rho\phi S)_t = \frac{\rho}{\sqrt{g}} \left[\frac{\sqrt{g}}{h_i^2} \left\{ \frac{k_i k_r}{\mu} \left(\frac{1}{h_i} P_{x_i} + \frac{\rho g}{h_i} z_{x_i} \right) \right\} \right]_{,i} + \frac{1}{h_i^2} \rho_{,i} \left\{ \frac{k_i k_r}{\mu} \left(\frac{1}{h_i} P_{x_i} + \frac{\rho g}{h_i} z_{x_i} \right) \right\} \quad . \tag{A-12}$$

For an elastic aquifer, the aquifer compressibility is given by the relation,

$$C_F = \frac{1}{\phi_o} \phi_p$$

which may be integrated to yield,

$$\phi = \phi_o \left[1 + C_F (P - P_o) \right] \tag{A-13}$$

where,

ϕ_o = Reference porosity

P_o = Reference pressure corresponding to the porosity ϕ_o .

Therefore,

$$\phi_t = C_F \phi_o P_t \quad . \tag{A-14}$$

Combining equations A-10, A-11 and A-14 and treating S as invariant with time,

$$(\rho\phi S)_t = \rho_o\phi_o S \left[\beta + 2C_F\beta\ (P - P_o) + C_F + C_F\alpha\ \frac{C-C_o}{\rho_o}\right] P_t$$

$$+ \alpha\phi_o S \left[1 + C_F\ (P - P_o)\right] C_t$$

C_F and β being of the same order of magnitude, the product,

$C_F\beta\ (P - P_o) \ll \beta$ for small pressure changes,

$C_F\alpha\ \frac{c - c_o}{\rho_o} \ll C_F$ for small changes in concentration and

$C_F\ (P - P_o) \ll 1$ for small pressure changes.

Therefore, for small pressure and concentration changes, equation A-12 may be written as,

$$\frac{1}{\rho}[\rho_o\phi_o S\ (\beta + C_F)\ P_t + \alpha\phi_o S\ C_t\ ] = \frac{1}{\sqrt{g}}\left[\frac{\sqrt{g}}{h_i^2}\left\{\frac{k_i k_r}{\mu}\left(\frac{1}{h_i}P_{x_i} + \frac{\rho g}{h_i}z_{x_i}\right)\right\}\right]_{,i}$$

$$+ \frac{1}{\rho h_i}\rho_{,i}\left\{\frac{k_i k_r}{\mu}\left(\frac{1}{h_i}P_{x_i} + \frac{\rho g}{h_i}z_{x_i}\right)\right\} \quad . \qquad \text{(A-15)}$$

For axisymmetric flow towards a well (neglecting the effect of partial penetration) in a completely saturated isotropic aquifer, equation A-15 reduces to,

$$\frac{1}{r}\left\{\frac{\rho r k}{\mu}\left(P_r + \rho g\ z_r\right)\right\}_r + \left\{\frac{\rho r k}{\mu}\left(P_z + \rho g\right)\right\}_z =$$

$$\rho_o\phi_o\ (\beta + C_F)\ P_t + \alpha\phi_o\ C_t \qquad \text{(A-16)}$$

which is the required flow equation.

Choosing L_o, ρ_o, k_o, μ_o, P_o and t_o as the scaling factors for length, density, permeability, dynamic viscosity, pressure or compressibility and time respectively, such that,

$$P_o = g\rho_o L_o \quad \text{and} \quad t_o = \frac{\mu_o L_o}{g\rho_o k_o} = \frac{\mu_o L_o^2}{P_o k_o} \quad ,$$

equation A-16 reduces to the following dimensionless form,

$$\phi_o \, (\bar{\beta} + \bar{C}_F) \, \bar{P}_{\bar{t}} + \alpha\phi_o \, \bar{C}_{\bar{t}} = \frac{\bar{\rho}\,\bar{k}}{\bar{\mu}\,\bar{r}} \, [\, \bar{P}_{\bar{r}} + \bar{\rho}\, \bar{z}_{\bar{r}} \,] +$$

$$[\, \frac{\bar{\rho}\,\bar{k}}{\bar{\mu}} \, \bar{P}_{\bar{r}} + \bar{\rho}\, \bar{z}_{\bar{r}} \,]_{\bar{r}} + [\, \frac{\bar{\rho}\,\bar{k}}{\bar{\mu}} \, \bar{P}_{\bar{z}} + \bar{\rho} \,]_{\bar{z}} \qquad \text{(A-17)}$$

where the bar denotes a dimensionless variable.

APPENDIX B

DERIVATION OF THE CONVECTIVE DISPERSION EQUATION

In a manner similar to the one adopted for the derivation of the flow equation, the convective-dispersion equation can be obtained by combining the mass-balance equation for the tracer with an equation that gives the mass flux of the tracer on a macroscopic scale.

EQUATION FOR MASS BALANCE:

Considering mass-balance for the k^{th} constituent of the tracer over a control volume D, with $\vec{n}$ as the unit outward normal to the boundary ∂D of D,

$$\int_{\partial D} J_i^k \phi S n_i \, d\sigma = - \left[\int_D C^k \phi S \, dv \right]_t + \sum_{m=1}^{s} \int_D R_m'^k \, dv - \int_D W'^k \delta \, dv \qquad (B\text{-}1)$$

where,

J_i^k = Component of the macroscopic mass-flux of tracer constituent k in i direction - $(ML^{-2}T^{-1})$

C^k = Mass concentration of the tracer constituent k - (ML^{-3})

$R_m'^k$ = Rate of production or consumption of the tracer constituent k in the m^{th} reaction - $(ML^{-3}T^{-1})$

$W'^k \delta$ = Cumulative equivalent of all the sources or sinks within the control volume

$$= \sum_{j=1}^{r} Q'^k (x_{1j}, x_{2j}, x_{3j}) \, C_p^k \, \delta (x_1 - x_{1j}) \cdot$$

$$\delta (x_2 - x_{2j}) \, \delta (x_3 - x_{3j}) \qquad - (ML^{-3}T^{-1})$$

C_p^k = Mass concentration of tracer constituent k in the

source or sink - (ML^{-3}) ,

and other symbols are as defined in Appendix A.

Using the divergence theorem,

$$\int_D \{ (J_i^k \phi S)_{,i} + (C^k \phi S)_t - \sum_{m=1}^{s} R'^k_m + Q'^k C^k_p d_{\not p} \} d\forall = 0 \quad \forall \not p \qquad (B\text{-}2)$$

where,

$$d\not p \to \delta \quad \text{as} \quad \not p \to \infty \quad .$$

Noting that the integrand of B-2 is continuous and the region D is arbitrary and also letting $\not p \to \infty$,

$$(J_i^k \phi S)_{,i} + (C^k \phi S)_t - \sum_{m=1}^{s} R'^k_m + Q'^k C^k_p \delta = 0 \quad . \qquad (B\text{-}3)$$

Assuming that,

(i) There are no reactions going on in the system,

(ii) There is only one tracer constituent so that the superscript k may be dropped and,

(iii) There are no sources or sinks in the system,

equation B-3 reduces to,

$$\text{div}(J\phi S) = - (C\phi S)_t \qquad (B\text{-}4)$$

EQUATION FOR THE MACROSCOPIC TRACER MASS FLUX:

Assuming that Fick's law holds, it can be shown, Reddell and Sunada (1970) that on a macroscopic scale for an isotropic medium, in an orthogonal system of coordinates:

$$J_i = Cv_i - D_{ij} (\text{grad } C)^j - D_d T (\text{grad } C)^j \qquad (B\text{-}5)$$

where,

Cv_i = Convective component of the tracer mass flux.

D_{ij} = Dispersion coefficient which is a second rank covariant symmetric tensor.

D_d = Coefficient of molecular diffusion.

T = Reciprocal of the tortuosity tensor which is scalar for an isotropic medium.

By the rules for inner (scalar) product of a covariant and a contravarient tensor,

$$D_{ij} \ (\text{grad } C)^j = D_{ij} \ g^{jk} \ C_{,k} \quad . \tag{B-6}$$

It has been shown (Bachmat and Bear, 1964) that,

$$D_{ij} = a_{ij\ell m} \frac{v_\ell v_m}{V} \tag{B-7}$$

where,

$a_{ij\ell m}$ = Geometric dispersivity of the porous medium. For an isotropic medium, it is a fourth rank isotropic tensor.

v_ℓ, v_m = Velocity components,

V = Absolute velocity.

Being an isotropic tensor of fourth rank $a_{ij\ell m}$ may, in an orthogonal system of coordinates be expanded as follows:

$$a_{ij\ell m} = \lambda \ g_{ij} \ g_{\ell m} + B_1 g_{i\ell} \ g_{jm} + B_2 \ g_{im} \ g_{j\ell} \tag{B-8}$$

where,

g_{ij} , $g_{\ell m}$, $g_{i\ell}$, g_{jm} , g_{im} and $g_{j\ell}$ are components of the metric covariant tensor.

Therefore, using the symmetry property, so that $B_1 = B_2 = \mu$,

$$D_{ij} = \lambda\, g_{ij}\, V + 2\mu\, \frac{v_i v_j}{V} \quad . \tag{B-9}$$

Substituting B-9 and B-6 into B-5,

$$J_i = C\, v_i - (\lambda g_{ij} V + 2\mu\, \frac{v_i v_j}{V})\, g^{ik}\, C_{,k} - D_d T\, (\text{grad } C)^j$$

$$= C\, v_i - (\lambda \delta_i^k\, V\, C_{,k} + 2\mu\, \frac{v_i v_j}{V}\, \frac{1}{(h_j)^2}\, C_{,j}) - D_d\, T\, (\text{grad } C)^j$$

$$= C\, v_i - (\lambda\, V\, C_{,i} + 2\mu\, \frac{v_i v^k}{V}\, C_{,k}) - D_d\, T\, (\text{grad } C)^j \quad . \tag{B-10}$$

Therefore,

$$\text{div } (J\phi S) = \nabla_i\, (J^i \phi S) = \{\, C\, \nabla_i\, v^i \phi S + v^i \phi S\, \nabla_i C \,\} -$$

$$\frac{1}{\sqrt{g}}\, [\, \sqrt{g}\, \phi\, S\, g^{ij}\, \{\, \lambda\, V\, C_{,j} + 2\mu\, \frac{v_j v^k}{V}\, C_{,k} \,\}\,]_{,i}$$

$$- \text{div } \{\, D_d\, T\, (\text{grad } C)^j \,\} \quad .$$

But,

$$\text{div } \{\, D_d T\, (\text{grad } C)^j \,\} = \frac{1}{\sqrt{g}}\, \{\, \sqrt{g}\, g^{ij}\, D_d\, T\, C_{,j} \,\}_{,i} \quad \text{(Moller, 1972).}$$

Therefore,

$$\text{div } (J\phi S) = \frac{C}{\sqrt{g}} \left(\sqrt{g}\, v_j \phi S\, g^{ij} \right)_{,i} + g^{ij}\, v_j \phi S\, C_{,i} -$$

$$\frac{1}{\sqrt{g}} \left[\sqrt{g}\, \phi\, S\, g^{ij} \left\{ \lambda\, V\, C_{,j} + \frac{2\mu\, v_j v^k}{V} C_{,k} + \right. \right.$$

$$\left. \left. D_d\, T\, C_{,j} \right\} \right]_{,i}$$

$$= \frac{C}{\sqrt{g}} \left(\frac{\sqrt{g}\, \phi\, S\, v_i}{h_i^2} \right)_{,i} + \frac{v_i \phi S}{h_i^2} C_{,i} -$$

$$\frac{1}{\sqrt{g}} \left[\sqrt{g}\, \frac{\phi S}{h_i^2} \left\{ \lambda\, V\, C_{,i} + \frac{2\mu\, v_i v_j}{V\, h_j^2} C_{,j} + D_d\, T\, C_{,i} \right\} \right]_{,i} .$$

Setting $q_i = v_i \phi S$,

$$\text{div } (J\phi s) = \frac{C}{\sqrt{g}} \left(\frac{\sqrt{g}\, q_i}{h_i^2} \right)_{,i} + \frac{q_i}{h_i^2} C_{,i} -$$

$$\frac{1}{\sqrt{g}} \left[\frac{\sqrt{g}\, \phi S}{h_i^2} \left\{ \lambda\, V\, C_{,i} + 2\mu\, \frac{v_i v_j}{V\, h_j^2} C_{,j} + \right. \right.$$

$$\left. \left. D_d\, T\, C_{,i} \right\} \right]_{,i} . \qquad \text{(B-11)}$$

CONVECTIVE-DISPERSION EQUATION:

Substituting equation B-11 into B-4, separating derivatives of C and transferring terms,

$$(\phi S)_t + \frac{1}{\sqrt{g}} \left(\frac{\sqrt{g}\, q_i}{h_i^2} \right)_{,i} = - \frac{\phi S}{C} C_t - \frac{q_i}{C\, h_i^2} C_{,i} + \frac{1}{C\sqrt{g}} \cdot$$

$$\left[\frac{\sqrt{g}\, \phi S}{h_i^2} \left\{ \lambda\, V\, C_{,i} + \frac{2\mu\, v_i v_j}{V\, h_j^2} C_{,j} + D_d\, T\, C_{,i} \right\} \right]_{,i} \qquad \text{(B-12)}$$

where the summation is performed both on i and j, except in h_i^2 and h_j^2.

It is to be noted here that the L.H.S. of equations A-7 and B-12 are the same. Therefore, equating the R.H.S. of both and collecting like terms,

$$\left(\frac{\phi S}{C} C_t - \frac{\phi S}{\rho} \rho_t \right) = - q_i \left(\frac{1}{C\, h_i^2} C_{,i} - \frac{1}{\rho\, h_i^2} \rho_{,i} \right) +$$

$$\frac{1}{C\sqrt{g}} \left[\frac{\sqrt{g}\, \phi S}{h_i^2} \left\{ \lambda\, V\, C_{,i} + \frac{2\mu\, v_i v_i}{V\, h_j^2} C_{,j} + D_d\, T\, C_{,i} \right\} \right]_{,i}$$

or $$\phi S \left[C_t - \frac{C}{\rho} \rho_t \right] = \frac{1}{\sqrt{g}} \left[\frac{\sqrt{g}\, \phi S}{h_i^2} \left\{ \lambda\, V\, C_{,i} + \frac{2\mu\, v_i v_j}{V\, h_j^2} C_{,j} + \right. \right.$$

$$\left. \left. D_d\, T\, C_{,i} \right\} \right]_{,i} - \frac{q_i}{h_i^2} \left[C_{,i} + \frac{C}{\rho} \rho_{,i} \right] \quad . \qquad \text{(B-13)}$$

Substituting values of ρ_t and $\rho_{,i}$ from equation A-11 and transferring terms,

$$\phi S \left(C_t - \frac{C}{\rho} \beta\, \rho_o\, P_t - \frac{C}{\rho} \alpha\, C_t \right) = DD_i - \frac{q_i}{h_i^2} \left[C_{,i} - \right.$$

$$\left. \frac{C}{\rho} \beta\, \rho_o\, P_{,i} - \frac{C}{\rho} \alpha\, C_{,i} \right]$$

where,

$$DD_i = \frac{1}{\sqrt{g}} \left[\frac{\sqrt{g}\, \phi S}{h_i^2} \left\{ \lambda\, V\, C_{,i} + \frac{2\mu\, v_i v_j}{V\, h_j^2} C_{,j} + D_d\, T\, C_{,i} \right\} \right]_{,i}$$

Therefore,

$$C_t = \frac{\rho}{\rho-\alpha C}\frac{DD_i}{\phi S} - \frac{v_i}{h_i^2}C_{,i} + \frac{\rho_o C\beta}{\rho-\alpha C}\left(P_t + \frac{v_i}{h_i^2}P_{,i}\right) \quad . \tag{B-14}$$

Assuming that,

(i) Medium is completely saturated so that S=1,

(ii) Terms containing fluid compressibility and the derivatives of pressure are small as compared to the other terms and so may be neglected,

equation B-14 reduces to,

$$C_t = \frac{\rho}{\rho-\alpha C}\frac{1}{\phi\sqrt{g}}\left[\frac{\sqrt{g}\,\phi}{h_i^2}\left\{\lambda V C_{,i} + \frac{2\mu\, v_i v_j}{V h_j^2}C_{,j} + D_d T C_{,i}\right\}\right]_{,i} - \frac{v_i}{h_i^2}C_{,i} \tag{B-15}$$

This is the general convective-dispersion equation for an isotropic, saturated porous medium.

For axisymmetric flow towards a well, equation B-15 transforms as follows:

$$C_t = \frac{\rho}{\rho-\alpha C}\left[\frac{1}{\phi r}\left\{\phi r\left(\lambda V + 2\mu\frac{u^2}{V}\right)C_r + \frac{2\mu\, uv}{V}C_z + D_d T C_r\right\}_r + \frac{1}{\phi}\left\{\phi\left(\lambda V + \frac{2\mu\, v^2}{V}\right)C_z + \frac{2\mu\, uv}{V}C_r + D_d T C_z\right\}_z\right] - uC_r - vC_z \tag{B-16}$$

where u and v are the velocity components in r and z directions respectively.

Also for an isotropic medium,

$\lambda = a_{II}$ = Lateral dispersivity of the medium and,

$\mu = (a_I - a_{II})/2$

where,

a_I = Longitudinal dispersivity of the medium,

$D_T = \lambda V = a_{II} V$ = Coefficient of lateral dispersion,

$2\mu V = (a_I - a_{II})\, V = D_L - D_T$

$D_L = a_I V$ = Coefficient of longitudinal dispersion.

Therefore, the expressions for the coefficients of hydrodynamic dispersion may be written as follows:

$$\left.\begin{aligned} D^*_{11} &= \lambda V + 2\mu \frac{u^2}{V^2} + D_d T \\ &= D_T + (D_L - D_T) \frac{u^2}{V^2} + D_d T \\ D^*_{22} &= \lambda V + 2\mu \frac{v^2}{V^2} + D_d T \\ &= D_T + (D_L - D_T) \frac{v^2}{V^2} + D_d T \\ D^*_{12} &= D^*_{21} = \frac{2\mu\, uv}{V} = (D_L - D_T) \frac{uv}{V^2} \end{aligned}\right\} \quad \text{(B-17)}$$

Using the above definitions, equation B-16 may be written as,

$$C_t = \frac{\rho}{\rho - \alpha C} \left[\frac{1}{\phi r} \{ \phi r \, (D^*_{11} C_r + D^*_{12} C_z) \}_r + \frac{1}{\phi} \{ \phi \, (D^*_{22} C_z + D^*_{12} C_r) \}_z \right] - u C_r - v C_z \quad . \quad \text{(B-18)}$$

Choosing ρ_o , V_o and D_o as the scaling factors for concentration, velocity and the coefficients of hydrodynamic dispersion or diffusion, in addition to those adopted for non-dimensionalizing the flow equation, such that,

$$V_o = \frac{L_o}{T_o} = \frac{g\rho_o k_o}{\mu_o}$$

and

$$D_o = \frac{L_o^2}{T_o}$$

equation B-18 reduces to the following dimensionless form,

$$\bar{C}_{\bar{t}} = \frac{\bar{\rho}}{\phi(\bar{\rho}-\alpha\bar{C})} \left[\frac{1}{\bar{r}} \{ \phi\bar{r} \, (\bar{D}_{11} \, \bar{C}_{\bar{r}} + \bar{D}_{12} \, \bar{C}_{\bar{z}}) \}_{\bar{r}} + \right.$$

$$\left. (\bar{D}_{22} \, \phi \, \bar{C}_{\bar{z}} + \bar{D}_{12} \, \phi \, \bar{C}_{\bar{r}})_{\bar{z}} \right] - \bar{u} \, \bar{C}_{\bar{r}} - \bar{v} \, \bar{C}_{\bar{z}} \qquad \text{(B-19)}$$

where the bar denotes dimensionless variables.

APPENDIX C

FINITE ELEMENT FORMULATION FOR THE FLOW EQUATION:

As shown in section 3.5, the flow equation reduces to the following form,

$$\frac{1}{r}(rSH_r)_r + (SH_z)_z - y_t = 0 \qquad \text{(C-1)}$$

where the subscript denotes derivative with respect to that variable. Following the Galerkin approach with arbitrary weighting functions W_p, ($p = i,j,k$) and equating the integrated values of the weighted residuals to zero, the following equations are obtained,

$$\iiint_v W_p \left[\frac{1}{r}(rSH_r)_r + (SH_z)_z - y_t \right] r\, dr\, d\theta\, dz = 0 \quad . \qquad \text{(C-2)}$$

Using divergence theorem to reduce the order of differentials and collecting the resulting volume and surface integrals separately, equation C-2 transforms as follows:

$$\iiint_v \left[SH_r (W_p)_r + SH_z (W_p)_z + W_p y_t \right] r\, dr\, d\theta\, dz =$$

$$\iint_S W_p SH_r n^1\, dS + \iint_s W_p SH_z n^3\, dS \qquad \text{(C-3)}$$

where n^1 and n^3 are the unit outward normals to the surface dS.

Referring to Fig. C-1 where the flow region has been shown with all its bounding surfaces and assuming that the boundaries c_4 and c_5 lie on the same vertical surface, the following boundary conditions will

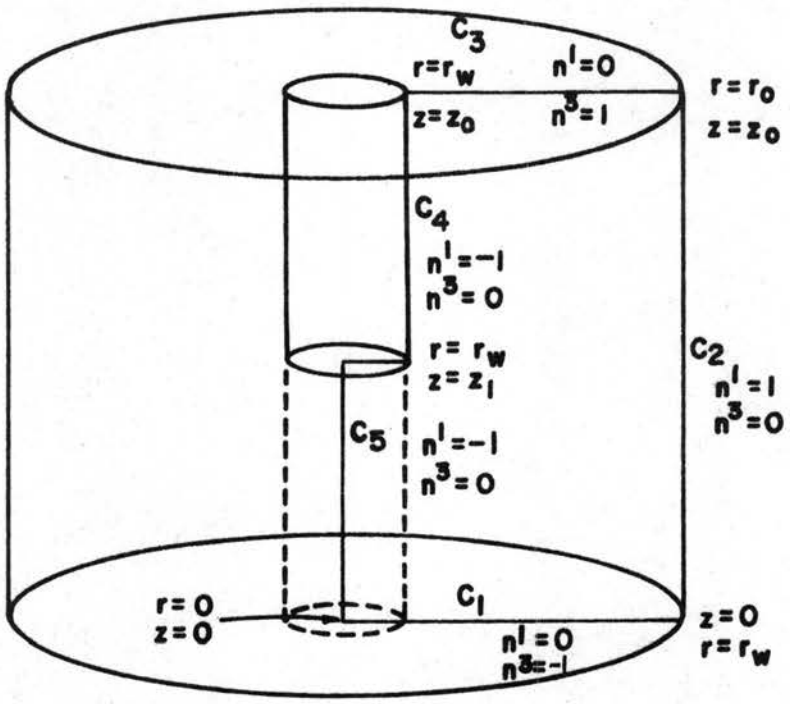


Fig. C.1 Schematic of Flow Boundaries

apply to the problem under investigation:

(i) c_1 and c_2 are geometric boundaries where the values of H are specified as,

$$H = H_i(r,z) \qquad \forall \quad t \geq 0 \quad .$$

As will be seen in subsequent discussion, prior knowledge of the R.H.S. of equation C-3 is not necessary for such boundaries.

(ii) c_3 and c_5 are natural boundaries, the former being the upper confining layer of the flow region and the latter being a vertical stream line due to radial symmetry. Thus,

$$SH_r = 0 \qquad \forall \quad t \geq 0 \qquad \text{along} \quad c_5$$

$$SH_z = 0 \qquad \forall \quad t \geq 0 \qquad \text{along} \quad c_3 \quad .$$

It, therefore, follows that the R.H.S. of equation C-3 reduces to zero on both these boundaries.

(iii) c_4 is the well face so that,

$$SH_z = 0 \qquad \forall \quad t \geq 0$$

and $$SH_r = -\rho q \qquad \forall \quad t \geq 0 \quad .$$

In order to apply equation C-3 to all the elements in the flow region, it is better for convenience of numerical computation, to work in terms of local coordinates referred to the centroid of each element as the origin. Thus introducing the above boundary conditions for any triangular element m , whose centroid is represented by the global coordinates $\bar{r}^m$ and $\bar{z}^m$, equation C-3 transforms as follows:

$$\iint_{R^m} [\, SH_\xi \, (W_p)_\xi + SH_\eta \, (W_p)_\eta + W_p \, y_t \,] \, (\bar{r}^m + \xi) \, d\xi \, d\eta =$$

$$\int_{S_2^m} W_p \, \rho q \, r_w \, d\eta + [R] \qquad \text{(C-4)}$$

where,

[R] refers to the unknown value of the R.H.S. of equation C-3 for the geometric boundaries and is zero everywhere except on the surfaces c_1 and c_2 ,

R^m refers to the area of the m^{th} element,

S_2^m refers to the boundary of the m^{th} element that lies along the well face and the integral along S_2^m is zero everywhere except the well boundary c_4 ,

$\xi = r - \bar{r}^m$,

$\eta = z - \bar{z}^m$

and, taking advantage of radial symmetry, the integral with respect to θ has been omitted from both the sides.

Assuming now, that over any triangular element with local coordinates of vertices as (ξ_i, η_i) , (ξ_j, η_j) and (ξ_k, η_k) , the flow parameter H may be represented by a first order polynomial,

$$H = \alpha_1 + \alpha_2 \xi + \alpha_3 \eta \qquad \text{(C-5)}$$

where α_1 , α_2 and α_3 are unknown coefficients, sometimes referred to as generalized coordinates. Using Cramer's rule to compute the values of these coefficients in terms of the nodal point values H_i , H_j and H_k , equation C-5 yields,

$$H = [A] \{H\}^m \qquad \text{(C-6)}$$

where,

$$\left.\begin{aligned} [A] &= \text{shape function} \\ &= [\, A_i \quad A_j \quad A_k \,] \\ A_p &= (a_{1p} + a_{2p}\xi + a_{3p}\eta)/2A^m \qquad p=i,j,k \\ a_{1i} &= \xi_j\eta_k - \eta_j\xi_k \\ a_{2i} &= \eta_j - \eta_k \\ a_{3i} &= \xi_k - \xi_j \end{aligned}\right\} \qquad \text{(C-7)}$$

and values of a_{1j} , a_{2j} , a_{3j} , a_{1k} , a_{2k} and a_{3k} follow in cyclic sequence.

$$2A^m = \begin{bmatrix} 1 & \xi_i & \eta_i \\ 1 & \xi_j & \eta_j \\ 1 & \xi_k & \eta_k \end{bmatrix} \quad , \qquad \text{(C-8)}$$

Similarly, assuming that y also varies linearly over the area of an element, it can be shown that,

$$y = [A]\,\{y\}^m \qquad \text{(C-9)}$$

and

$$y_t = [A]\,\{y_t\}^m \qquad \text{(C-10)}$$

In view of the continuity property of the shape function [A] , it is expedient to specify that,

$$W_p = A_p \qquad p=i,j,k \quad .$$

Substituting the values of H , A_p and y_t from equations C-6, C-7 and C-10, equation C-4 yields,

$$\iint_{R^m} \left(\left[S \right][A]_{\xi} (A_p)_{\xi} + S \left[A \right]_{\eta} (A_p)_{\eta} \right] \{H\}^m + A_p \left[A \right] \{y_t\}^m \right) \cdot$$

$$(\bar{r}^m + \xi)\, d\xi\, d\eta = \int_{S_2^m} A_p\, \rho q\, rw\, d\eta + [R] \quad . \qquad \text{(C-11)}$$

Recognizing that,

$$\left.\begin{aligned} [A]_{\xi} &= \frac{1}{2A^m} \left[a_{2i} \quad a_{2j} \quad a_{2k} \right] \\ [A]_{\eta} &= \frac{1}{2A^m} \left[a_{3i} \quad a_{3j} \quad a_{3k} \right] \\ [A_p]_{\xi} &= \frac{a_{2p}}{2A^m} \\ [A_p]_{\eta} &= \frac{a_{3p}}{2A^m} \end{aligned}\right\} \qquad \text{(C-12)}$$

,

evaluating the integrals and writing down three separate equations with the three weighting functions A_i , A_j and A_k in matrix form, the following system of equations is obtained,

$$\left[\left[SA \right] + \left[SC \right] \right] \{H\}^m + \left[\left[SAA \right] + \left[SALPHA \right] + \left[SBETA \right] + \left[SGAMA \right] \right.$$

$$\left. + \left[STHETA \right] \right] \{y_t\}^m = \left[Q \right] + \left[R \right] \qquad \text{(C-13)}$$

where,

$$[SA] = \frac{s\ \bar{r}^m\ A}{4\ A^m\ A^m} \cdot [A_{mn}]$$

A = Area of the element .

$$A_{mn} = a_{2m}\ a_{2n} \qquad n=i,j,k\ ;\ m=i,j,k$$

$$[SC] = \frac{s\ \bar{r}^m\ A}{4\ A^m\ A^m}\ [C_{mn}]$$

$$C_{mn} = a_{3m}\ a_{3n}$$

$$[SAA] = \frac{\bar{r}^m}{4\ A^m\ A^m}\ [\phi_{mn}]$$

$$[\phi_{mn}] = a_{1m}\ a_{2n}\ A + a_{2m}\ a_{1n}\ XISQ + (a_{3m}\ a_{2n} + a_{2m}\ a_{3n})\ XITA + a_{3m}\ a_{3n}\ TASQ$$

$$XISQ = \iint_{R^m} \xi^2\ d\xi\ d\eta$$

$$XITA = \iint_{R^m} \xi\ \eta\ d\xi\ d\eta$$

$$TASQ = \iint_{R^m} \eta^2\ d\xi\ d\eta$$

$$[SALPHA] = \frac{1}{4\ A^m\ A^m}\ [\alpha_{mn}]$$

$$\alpha_{mn} = (a_{2m}\ a_{1n} + a_{1m}\ a_{2n})\ XISQ + (a_{3m}\ a_{1n} + a_{1m}\ a_{3n})XITA$$

$$[SBETA] = \frac{EXXET}{4\ A^m\ A^m}\ [\beta_{mn}]$$

$$\beta_{mn} = a_{2m}\ a_{3n} + a_{3m}\ a_{2n}$$

$$EXXET = \iint_{R^m} \xi^2\ \eta\ d\xi\ d\eta$$

$$[SGAMA] = \frac{EXXX}{4\ A^m\ A^m}\ [\gamma_{mn}]$$

$$\gamma_{mn} = a_{2m}\ a_{2n}$$

$$EXXX = \iint_{R^m} \xi^3\ d\xi\ d\eta$$

$$[STHETA] = \frac{EXETT}{4\ A^m\ A^m}\ [\Theta_{mn}]$$

$$\Theta_{mn} = a_{3m}\ a_{3n}$$

$$EXETT = \iint_{R^m} \xi\ \eta^2\ d\xi\ d\eta$$

$$[Q] = \begin{bmatrix} q_i^* \\ q_j^* \end{bmatrix} \quad ,$$

i and j refer respectively to the lower and upper nodes of element m lying along the well face and,

$$q_i^* = \frac{r_w\ \rho q}{2}\ (\eta_j - \eta_i)$$

$$q_j^* = \frac{r_w\ \rho q}{2}\ (\eta_j - \eta_i) \quad .$$

In a more compact symbolic form equation C-13 may be expressed as,

$$[FSL]\ \{H\}^m + [FPLE]\ \{y_t\}^m = [Q]^m + [R]^m \qquad \text{(C-14)}$$

where,

$$[FSL] = [SA] + [SC] \qquad \text{and}$$

$$[FPLE] = [SAA] + [SALPHA] + [SBETA] + [SGAMA] + [STHETA] \quad .$$

In order to get the contributions pertaining to all the nodes in the system, matrix equations similar to C-14 have to be combined for all

the elements in the layout following the general assembly process of the finite element formulation. Any node common to two or more elements will have non-zero contributions from all such elements and no contribution from the remaining elements. This results in the following system of equations,

$$[SK]\ \{H\} + [PK]\ \{y_t\} - [QK] = [R] \quad . \tag{C-15}$$

Considering the solution in the time domain, it follows from the discussion in section 3.6 that equation C-15 may be written as,

$$[SK]\ \{H\} + E \cdot [PK]\ \{H_t\} - [QK] = [R] \quad . \tag{C-16}$$

Assuming a linear variation of H over a small increment of time Δt, the shape function $[N]$ for the time domain formulation is given by,

$$[N] = [\ N_0 \quad N_1\ ]$$

$$= \left[\ \left(1 - \frac{t}{\Delta t}\right) \qquad \frac{t}{\Delta t}\ \right]$$

where the subscripts $_0$ and $_1$ refer to the time levels $_0$ and Δt respectively. Using the Galerkin approach with N_1 as the weighting function, the following set of equations is obtained,

$$\int_0^{\Delta t} N_1\ (\ [SK]\ \{H\} + E \cdot [PK]\ \{H_t\} - [QK] - [R]\ )\ dt = 0 \quad .$$

Recognizing that,

$$\{H_t\} = \frac{1}{\Delta t}\ [\ 1 \quad -1\ ]\ \begin{Bmatrix} \{H\}_0 \\ \{H\}_1 \end{Bmatrix} \qquad \text{and}$$

$$\{H\} = \frac{1}{\Delta t}\ [\ (\Delta t - t) \quad t\ ]\ \begin{Bmatrix} \{H\}_0 \\ \{H\}_1 \end{Bmatrix} \quad ,$$

the above integration yields,

$$\left[\frac{2}{3} [SK] + \frac{E}{\Delta t} [PK] \right] \{H\}_1 = [R] + [QK] + \left[\frac{E}{\Delta t} [PK] - \frac{1}{3} [SK] \right] \{H\}_0 \quad . \tag{C-17}$$

As an alternative to Galerkin, sub-domain method, Crandall (1956) may be used for the time-domain solution for computational simplicity. Thus,

$$\int_0^{\Delta t} \left([SK] \{H\} + E \cdot [PK] \{H_t\} - [QK] - [R] \right) dt = 0 \quad . \tag{C-18}$$

Evaluating the integral using the same interpolation function for H , results in the following:

$$\left[\frac{1}{2} [SK] + \frac{E}{\Delta t} \cdot [PK] \right] \{H\}_1 = [R] + [QK] + \left[\frac{E}{\Delta t} \cdot [PK] - \frac{1}{2} [SK] \right] \{H\}_0 \quad . \tag{C-19}$$

APPENDIX D

FINITE ELEMENT FORMULATION FOR THE CONVECTIVE-DISPERSION EQUATION:

As shown in section 3.8, the convective-dispersion equation reduces to the following form:

$$\frac{1}{r}\,(r\,D_{rr}\,C_r + r\,D_{rz}\,C_z)_r + (D_{zz}\,C_z + D_{rz}\,C_r)_z - uC_r - vC_z - C_t = 0 \qquad \text{(D-1)}$$

where D_{rr} , D_{rz} and D_{zz} are the three coefficients of hydrodynamic dispersion and everywhere else the subscript denotes derivative with respect to that variable. Following the Galerkin approach with arbitrary weighting functions W_p , $(p=i,j,k)$ and equating the integrated values of the weighted residuals to zero, the following equations are obtained,

$$\iiint_V W_p \left[\frac{1}{r} \left(r\,D_{rr}\,C_r + r\,D_{rz}\,C_z \right)_r + (D_{zz}\,C_z + D_{rz}\,C_r)_z - uC_r \right.$$

$$\left. - vC_z - C_t \right] r\,dr\,d\theta\,dz = 0 \qquad . \qquad \text{(D-2)}$$

Using divergence theorem to reduce the order of differentials and collecting the resulting volume and surface integrals separately, equation D-2 transforms as follows:

$$\iiint_V \left[(W_p)_r\,(D_{rr}\,C_r + D_{rz}\,C_z) + (W_p)_z\,(D_{zz}\,C_z + D_{rz}\,C_r) \right.$$

$$\left. + W_p\,(uC_r + vC_z + C_t) \right] r\,dr\,d\theta\,dz =$$

$$\iint_S W_p\,(D_{rr}\,C_r + D_{rz}\,C_z)\,n^1 dS + \iint_S W_p\,(D_{zz}\,C_z + D_{rz}\,C_r)\,n^3 dS \qquad \text{(D-3)}$$

where n^1 and n^3 are the unit outward normals to the surface dS. Referring to Fig. C-1 and assuming that the boundaries c_4 and c_5 lie on the same vertical surface, the following boundary conditions will apply to the problem under investigation:

(i) c_1 and c_2 are geometric boundaries where the values of C are specified as,

$$C = C_i(r,z) \qquad \forall \qquad t \geq 0 \quad .$$

As will be seen in subsequent discussion, prior knowledge of the R.H.S. of equation D-3 is not necessary for such boundaries.

(ii) c_3 and c_5 are natural boundaries, the former being the upper confining layer of the flow region and the latter a vertical stream line due to radial symmetry. Thus,

$$D_{rr}\, C_r + D_{rz}\, C_z = 0 \qquad \forall \qquad t \geq 0 \quad \text{along } c_5$$

$$D_{rz}\, C_r + D_{zz}\, C_z = 0 \qquad \forall \qquad t \geq 0 \quad \text{along } c_3 \quad .$$

It, therefore, follows that the R H.S. of equation D-3 reduces to zero on both these boundaries.

(iii)c_4 is the well face so that,

$$D_{rz}\, C_r + D_{zz}\, C_z = 0 \qquad \forall \qquad t \geq 0$$

and $$D_{rr}\, C_r + D_{rz}\, C_z = qC\left(\frac{1}{\phi} - 1\right) \qquad \forall \qquad t \geq 0 \quad .$$

For element to element application of equation D-3, it is more convenient to work in terms of local coordinates referred to the centroid of each element as the origin. Thus introducing the above boundary conditions for any triangular element m, whose centroid is represented by the global coordinates $\bar{r}^m$ and $\bar{z}^m$, equation D-3 transforms as follows:

$$\iint_{R^m} \left[(W_p)_\xi \left(D_{rr} C_\xi + D_{rz} C_\eta\right) + (W_p)_\eta \left(D_{zz} C_\eta + D_{rz} C_\xi\right) + W_p \left(uC_\xi + vC_\eta + C_t\right) \right] \left(\bar{r}^m + \xi\right) d\xi \, d\eta$$

$$= -\int_{S_2^m} W_p \, q \, C \left(\frac{1}{\phi} - 1 \right) r_w \, d\eta + [R] \qquad \text{(D-4)}$$

where,

R^m refers to the area of the m^{th} element,

S_2^m refers to the boundary of the m^{th} element that lies along the well face and the integral along S_2^m is non-zero only along the well boundary c_4 ,

$[R]$ refers to the unknown values of the R.H.S. of equation D-3 for the geometric boundaries. Obviously $[R]$ is a null matrix everywhere except along the surfaces c_1 and c_2 ,

$\xi = r - \bar{r}^m$,

$\eta = z - \bar{z}^m$,

and, taking advantage of radial symmetry, the integral with respect to θ has been omitted from both the sides.

Assuming now, that over any triangular element with local coordinates of vertices as (ξ_i,η_i) , (ξ_j,η_j) and (ξ_k,η_k) , the concentration C may be represented by a first order polynomial,

$$C = \alpha_1 + \alpha_2 \xi + \alpha_3 \eta \quad , \qquad \text{(D-5)}$$

where,

α_1 , α_2 and α_3 are unknown coefficients, sometimes referred to as generalized coordinates. Using Cramer's rule to compute the values of these coefficients in terms of the nodal point values C_i , C_j and

C_k , equation D-5 yields,

$$C = [A]\ \{C\}^m \tag{D-6}$$

where,

[A] = shape function.

This shape function is exactly the same as was obtained for the flow equation in Appendix C. Using this shape function as the weighting function also and substituting values of C , C_t and the derivatives of [A] in equation D-4, the following set is obtained,

$$\iint_{R^m} \{((A_p)_\xi [D_{rr}\ [A]_\xi + D_{rz}\ [A]_\eta] + (A_p)_\eta\ [D_{zz}\ [A]_\eta + D_{rz}\ [A]_\xi]$$

$$+ u\ [A]_\xi\ A_p + v\ [A]_\eta\ A_p\ )\ (\bar{r}^m + \xi)\ d\xi\ d\eta\ \}\ \{C\}^m$$

$$+ \iint_{R^m} \{\ A_p\ [A]\ (\bar{r}^m + \xi)\ d\xi\ d\eta\ \}\ \{C_t\}^m$$

$$= - \int_{S^m} A_p\ [A]\ q\ (\frac{1}{\phi} - 1)\ r_w\ \{C\}^m\ d\eta + [R] \quad . \tag{D-7}$$

Evaulating integrals and writing down three separate equations with the three weighting functions A_i , A_j and A_k in matrix form, the following system of equations is obtained,

$$[\ [SA] + [SB] + [SC] + [SF] + [SG] + [SH] + [SI]\ ]\ \{C\}^m$$

$$+ [\ [SAA] + [SALPHA] + [SBETA] + [SGAMA] + [STHETA]\ ]\ \{C_t\}^m$$

$$= - [Q] + [R] \tag{D-8}$$

where,

$$[SA] = \frac{D_{rr}\ \bar{r}^m\ A}{4\ A^m\ A^m}\ [A_{mn}]$$

A , A^m and A_{mn} have the same values as defined in

Appendix C.

$$[SB] = \frac{D_{rz}\ \bar{r}^m\ A}{4\ A^m\ A^m}\ [B_{mn}]$$

$$B_{mn} = a_{3m}\ a_{2n} + a_{2m}\ a_{3n} \qquad n=i,j,k \ ; \quad m=i,j,k$$

$$[SC] = \frac{D_{zz}\ \bar{r}^m\ A}{4\ A^m\ A^m}\ [C_{mn}]$$

C_{mn} has the same values as defined in Appendix C.

$$[SF] = \frac{u}{4\ A^m\ A^m}\ [F_{mn}]$$

$$F_{mn} = a_{2m}\ a_{2n}\ XISQ + a_{3m}\ a_{2n}\ XITA$$

$$[SG] = \frac{v}{4\ A^m\ A^m}\ [G_{mn}]$$

$$G_{mn} = a_{2m}\ a_{3n}\ XISQ + a_{3m}\ a_{3n}\ XITA$$

$$[SH] = \frac{u\ \bar{r}^m\ A}{4\ A^m\ A^m}\ [H_{mn}]$$

$$H_{mn} = a_{1m}\ a_{2n}$$

$$[SI] = \frac{v\ \bar{r}^m\ A}{4\ A^m\ A^m}\ [I_{mn}]$$

$$I_{mn} = a_{1m}\ a_{3n}$$

[SAA] , [SALPHA] , [SBETA] , [SGAMA] and [STHETA] have the

same values as defined in Appendix C.

In a more compact symbolic representation, equation D-8 may be expressed as,

$$[SL]\ \{C\}^m + [PL]\ \{C_t\}^m = -\ [Q]^m + [R]^m \qquad \text{(D-9)}$$

where,

$$[SL] = [SA] + [SB] + [SC] + [SF] + [SG] + [SH] + [SI]$$

$$[PL] = [SAA] + [SALPHA] + [SBETA] + [SGAMA] + [STHETA]$$

$$[Q]^m = \begin{bmatrix} q_i^* \\ q_j^* \end{bmatrix} \quad ,$$

i and j refer respectively to the lower and upper nodes of element m lying along the well face. Evaluating the integral on the R.H.S. of equation D-7 along the well boundary,yields,

$$q_i^* = r_w\, q\, \left(\frac{1}{\phi} - 1\right) \left(\frac{C_i}{3} + \frac{C_j}{6}\right) (\eta_j - \eta_i)$$

$$q_j^* = r_w\, q\, \left(\frac{1}{\phi} - 1\right) \left(\frac{C_i}{6} + \frac{C_j}{3}\right) (\eta_j - \eta_i) \quad .$$

In order to get the contributions pertaining to all the nodes in the system, matrix equations similar to D-9 have to be combined for all the elements in the layout following the general assembly process of the finite element formulation. Any node common to two or more elements will have non-zero contributions from all such elements and no contribution from the remaining elements. This results in the following system of equations,

$$[SK]\ \{C\} + [PK]\ \{C_t\} + [QK] = [R] \quad . \qquad \text{(D-10)}$$

For the time domain solution, following exactly the same approach as was done for the flow equation, the following expression for the weighted residual is obtained,

$$\int_0^{\Delta t} N_1 \left([SK] \{C\} + [PK] \{C_t\} + [QK] - [R] \right) dt = 0 \quad . \text{(D-11)}$$

Substituting value of the weighting function N_1 from Appendix C, equation D-11 yields,

$$\left[\frac{2}{3} [SK] + \frac{1}{\Delta t} [PK] \right] \{C\}_1 = [R] - [QK] + \left[\frac{1}{\Delta t} [PK] - \frac{1}{3} [SK] \right] \{C\}_0 \quad . \text{(D-12)}$$

Alternatively, the sub-domain method gives,

$$\left[\frac{1}{2} [SK] + \frac{1}{\Delta t} [PK] \right] \{C\}_1 = [R] - [QK] + \left[\frac{1}{\Delta t} [PK] - \frac{1}{2} [SK] \right] \{C\}_0 \quad . \text{(D-13)}$$

APPENDIX E

Rayleigh-Ritz Formulation for the Convective-Dispersion Equation:

Assuming that ϕ , u , v , D_{11}^{*} , D_{12}^{*} and D_{22}^{*} are invariant over an element and that C_t is invariant over a single time-step, the convective-dispersion equation B-18 may be derived from a variational principle, provided there exists a reducing factor $A(r,z)$ which satisfies the following system of simultaneous first-order partial differential equations (Hildebrand, 1965),

$$\left.\begin{aligned} D_{rr}\, A_r + D_{rz}\, A_z &= \left(\frac{D_{rr}}{r} - u \right) A \\ D_{rz}\, A_r + D_{zz}\, A_z &= \left(\frac{D_{rz}}{r} - v \right) A \end{aligned}\right\} \qquad \text{(E-1)}$$

It can be seen that the common solution of these equations is,

$$A(r,z) = r \exp(\beta)$$

where,

$$\beta = \frac{v\, D_{rz} - u\, D_{zz}}{D_{zz}\, D_{rr} - D_{rz}^2}\, r + \frac{u\, D_{rz} - v\, D_{rr}}{D_{zz}\, D_{rr} - D_{rz}^2}\, z$$

$$= - \frac{ur + vz}{D_L + D_d\, T} \cdot \frac{\rho - \alpha C}{\rho} \qquad \text{(E-2)}$$

The corresponding J-functional is,

$$J = \iint_{R^m} \left[\frac{D_{rr}}{2} (C_r)^2 + D_{rz}\, C_r\, C_z + \frac{D_{zz}}{2} (C_z)^2 + C\, C_t \right] r\, e^{\beta}\, dr\, dz$$

$$+ \int_{S_2^m} r_w\, q \left(\frac{1}{\phi} - 1 \right) e^{\beta}\, \frac{C^2}{2}\, dS \qquad \text{(E-3)}$$

where the subscripts denote derivatives with respect to those variables, R^m represents the area of the m^{th} element, S_2^m is the well boundary, if any, included in the boundary of the m^{th} element, r_w is the well radius and,

$$q = \frac{Q_w}{2\pi\ r_w\ \text{PENETR}} \quad ,$$

Q_w being the well discharge.

To reduce the expression E-3 into a conveniently tractable minimizing problem, it is expedient to introduce a new concentration parameter ψ , such that,

$$\psi = C\ e^{\beta/2} \quad . \tag{E-4}$$

In terms of this parameter , ψ , equation E-3 transforms to,

$$J = \iint_{R^m} \left[\frac{D_{rr}}{2} (\psi_r)^2 + D_{rz} (\psi_r \cdot \psi_z) + \frac{D_{zz}}{2} (\psi_z)^2 + \psi \left(\frac{u}{2} \psi_r + \frac{v}{2} \psi_z \right) \right.$$

$$\left. + \psi^2 f(r,z) + \psi \psi_t \right] r\ dr\ dz + \int_{S^m} r_w\ q \left(\frac{1}{\phi} - 1 \right) \frac{\psi^2}{2}\ dS \tag{E-5}$$

and the convective-dispersion equation B-18 transforms to,

$$\psi_t + \left\{ 2\ f(r,z) - \frac{u}{2r} \right\} \psi = D_{rr}\ \psi_{rr} + 2D_{rz}\ \psi_{rz} + D_{zz}\ \psi_{zz}$$

$$+ \frac{D_{rr}}{r} \psi_r + \frac{D_{rz}}{r} \psi_z \tag{E-6}$$

where,

$$f(r,z) = \frac{D_{zz}\ u^2 + v^2\ D_{rr} - 2\ u\ v\ D_{rz}}{8\ (D_{rr}\ D_{zz} - D_{rz}^2)} \quad . \tag{E-7}$$

That equation E-6 is the Euler equation for the variational functional E-5 may be verified by equating the first variation of J to zero. Thus,

$$\delta J = \iint_{R^m} [\, D_{rr}\, \psi_r\, \delta\psi_r + D_{rz}\, \psi_r\, \delta\psi_z + D_{rz}\, \psi_z\, \delta\psi_r + D_{zz}\, \psi_z\, \delta\psi_z$$

$$+ \left(\frac{u}{2}\, \psi_r + \frac{v}{2}\, \psi_z \right) \delta\psi + \psi\, \frac{u}{2}\, \delta\psi_r + \psi\, \frac{v}{2}\, \delta\psi_z + 2\psi\, f(r,z)\, \delta\psi$$

$$+ \psi_t\, \delta\psi \,]\, r\, dr\, dz + \int_{S_2^m} r_w\, q \left(\frac{1}{\phi} - 1 \right) \psi\, \delta\psi\, dz = 0 \qquad . \text{(E-8)}$$

Using the divergence theorem equation E-8 yields (Ref. Fig. C-1),

$$\delta J = \iint_{R^m} [\, - \frac{1}{r} (r\, D_{rr}\, \psi_r)_r - \frac{1}{r} (r\, D_{rz} \psi_r)_z - \frac{1}{r} (r\, D_{rz} \psi_z)_r$$

$$- \frac{1}{r} (r\, D_{zz} \psi_z)_z + \frac{u}{2}\, \psi_r + \frac{v}{2}\, \psi_z - \frac{1}{r} (r\, \psi\, \frac{u}{2}\,)_r - \frac{1}{r} (r\, \psi\, \frac{v}{2}\,)_z$$

$$+ 2\psi\, f(r,z) + \psi_t \,]\, \delta\psi\, r\, dr\, dz + \int_{r_w}^{r_o} - (D_{rz} \psi_r + D_{zz} \psi_z + \psi\, \frac{v}{2}\,)$$

$$r\, dr\, \delta\psi \,\Big|_{z=o} + \int_{r_w}^{r_o} (D_{rz} \psi_r + D_{zz} \psi_z + \psi\, \frac{v}{2}\,)\, r\, dr\, \delta\psi \,\Big|_{z=z_o}$$

$$+ \int_{o}^{z_o} (D_{rr} \psi_r + D_{rz} \psi_z + \psi\, \frac{u}{2}\,)\, r\, dz\, \delta\psi \,\Big|_{r=r_o} + \int_{o}^{z_1} - (D_{rr} \psi_r$$

$$+ D_{rz} \psi_z + \psi\, \frac{u}{2}\,)\, r\, dz\, \delta\psi \,\Big|_{r=r_w} + \int_{z_1}^{z_o} - (D_{rr} \psi_r + D_{rz} \psi_z + \psi\, \frac{u}{2}\,)$$

$$r\, dz\, \delta\psi \,\Big|_{r=r_w} + \int_{z_1}^{z_o} r_w\, q \left(\frac{1}{\phi} - 1 \right) \psi\, dz\, \delta\psi \,\Big|_{r=r_w} \qquad . \text{(E-9)}$$

The boundary conditions, in terms of the variable ψ are,

(i) $D_{rr}\psi_r + D_{rz}\psi_z + u\frac{\psi}{2} = 0$ along the natural boundary c_5 ,

(ii) $D_{rz}\psi_r + D_{zz}\psi_z + v\frac{\psi}{2} = 0$ along the natural boundary c_3 ,

(iii) $D_{rr}\psi_r + D_{rz}\psi_z + \frac{u\psi}{2} - q\left(\frac{1}{\phi} - 1\right)\psi = 0$ along the natural boundary c_4 ,

(iv) $\delta\psi$ is zero along the geometric boundaries c_1 and c_2 .

Substituting these boundary conditions in E-9, it is seen that all the line integrals vanish. Therefore,

$$(r\,D_{rr}\psi_r)_r + (r\,D_{rz}\psi_r)_z + (r\,D_{rz}\psi_z)_r + (r\,D_{zz}\psi_z)_z - \frac{ur}{2}\psi_r - \frac{vr}{2}\psi_z + (r\,\psi\,\frac{u}{2})_r + (r\,\psi\,\frac{v}{2})_z - 2\psi\,r\,f(r,z) - r\,\psi_t = 0 \qquad \text{(E-10)}$$

which may be verified to be the same as the convective-dispersion equation E-6. Transforming to the local coordinate system equation E-5 becomes,

$$J = \iint_{R^m} \left[\frac{D_{rr}}{2}(\psi_\xi)^2 + D_{rz}\,\psi_\xi\,\psi_\eta + \frac{D_{zz}}{2}\psi_\eta^2 + \psi\left(\frac{u}{2}\psi_\xi + \frac{v}{2}\psi_\eta\right) + \psi^2 f(r,z) + \psi\,\psi_t\right](\xi + \bar{r}^m)\,d\xi\,d\eta + \int_{S_2^m} r_w\,q\left(\frac{1}{\phi} - 1\right)\frac{\psi^2}{2}\,d\eta \qquad \text{(E-11)}$$

Considering the minimization process,

$$J_{\psi_p} = \iint_{R^m} [\, D_{rr}\, \psi_\xi\, (\psi_\xi)_{\psi_p} + D_{rz} \{\, \psi_\xi\, (\psi_\eta)_{\psi_p} + \psi_\eta\, (\psi_\xi)_{\psi_p} \,\}$$

$p=i,j,k$

$$+ D_{zz}\, \psi_\eta\, (\psi_\eta)_{\psi_p} + \psi \{\, \frac{u}{2}\, (\psi_\xi)_{\psi_p} + \frac{v}{2}\, (\psi_\eta)_{\psi_p} \,\}$$

$$+ \psi_{\psi_p} \{\, \frac{u}{2}\, \psi_\xi + \frac{v}{2}\, \psi_\eta \,\} + \psi \{\, \frac{\rho-\alpha c}{\rho} \cdot \frac{u^2 + v^2}{4(D_L+D_d T)} \,\}\, \psi_{\psi_p}$$

$$+ \psi_t\, \psi_{\psi_p} \,]\, (\xi + \bar{r}^m)\, d\xi\, d\eta + \int_{S_2^m} r_w\, q\, (\, \frac{1}{\phi} - 1\,)\, \frac{\psi^2}{2}\, d\eta \Big|_{r=r_w} \qquad \text{(E-12)}$$

Introducing a shape function such that,

$$\psi = [A]\, \{\psi\} \qquad \text{(E-13)}$$

where [A] is as defined earlier and evaluating the surface and line integrals in equation E-12 separately, the following two systems of matrices are obtained:

(i) For the surface integral,

$$\frac{\bar{r}^m\, D_{rr}\, A}{4\, A^m\, A^m} [a_{2m}\, a_{2n}] + \frac{\bar{r}^m\, D_{rz}\, A}{4\, A^m\, A^m} [a_{3m}\, a_{2n} + a_{2m}\, a_{3n}]$$

$$+ \frac{\bar{r}^m\, D_{zz}\, A}{4\, A^m\, A^m} [a_{3m}\, a_{3n}] + \frac{u}{8\, A^m\, A^m} \{\, a_{2m}\, [a_{2n}\, XISQ + a_{3n}\, XITA] \,\}$$

$$+ \frac{v}{8\, A^m\, A^m} \{\, a_{3m}\, [a_{2n}\, XISQ + a_{3n}\, XITA] \,\}$$

$$+ \frac{u}{8\, A^m\, A^m} [a_{2m}\, a_{2n}\, XISQ + a_{3m}\, a_{2n}\, XITA]$$

$$+ \frac{v}{8\, A^m\, A^m} [a_{2m}\, a_{3n}\, XISQ + a_{3m}\, a_{3n}\, XITA]$$

$$+ \frac{u\,\bar{r}^m A}{8\,A^m A^m}\,[a_{1m}\,a_{2n} + a_{2m}\,a_{1n}] + \frac{v\,\bar{r}^m A}{8\,A^m A^m}\,[a_{1m}\,a_{3n} + a_{3m}\,a_{1n}]$$

$$+ \frac{\rho-\alpha c}{\rho} \cdot \frac{u^2 + v^2}{4(D_d T + D_L)} \{\, [SAA] + [SALPHA] + [SBETA] + [SGAMA]$$

$$+ [STHETA] \,\}\, \{\psi\}^m + \{\, [SAA] + [SALPHA] + [SBETA] + [SGAMA]$$

$$+ [STHETA] \,\}\, \{\psi_t\}^m \qquad \text{(E-14)}$$

where, $n=i,j,k$; $m=i,j,k$ and the symbols are as defined in Appendix C.

The expression E-14 may be represented in the following condensed symbolic form,

$$\{\, [SA] + [SB] + [SC] + [SD] + [SE] + [SF] + [SG] + [SH] + [SI]$$

$$+ \frac{\rho-\alpha c}{\rho} \quad \frac{u^2 + v^2}{4(D_d T + D_L)}\, [PL] \,\}\, \{\psi\}^m + [PL]\, \{\psi_t\}^m$$

or $$[SL]\, \{\psi\}^m + [PL]\, \{\psi_t\}^m \qquad \text{(E-15)}$$

where the matrices [SL] and [PL] are symmetric and refer to the m^{th} element.

(ii)Considering the contribution of the line integral between the two nodes i and j of the m^{th} element, which lie along the well face, the linear interpolation of ψ yields,

$$\psi = [\, 1 \quad n \,] \begin{bmatrix} 1 & 0 \\ -1/\ell & 1/\ell \end{bmatrix} \begin{Bmatrix} \psi_i \\ \psi_j \end{Bmatrix} \qquad \text{(E-16)}$$

where, η is the distance of the point to which the value ψ pertains, from the nodal point i, referred to as origin, and $\ell = \eta_j - \eta_i$, η_i being treated as zero. Thus, the line integral components are,

$$[J^m_{\psi_i}]_1 = \int_0^{\ell} r_w\, q \left(\frac{1}{\phi} - 1\right) \psi\, \psi_{\psi_i}\, d\eta$$

$$= r_w\, q \left(\frac{1}{\phi} - 1\right) \left(\frac{\psi_i}{3} + \frac{\psi_j}{6}\right) \ell$$

$$= q_i^*$$

and, similarly,

$$[J^m_{\psi_i}]_2 = r_w\, q \left(\frac{1}{\phi} - 1\right) \left(\frac{\psi_i}{6} + \frac{\psi_j}{3}\right) \ell$$

$$= q_j^* \quad .$$

This could be represented by a column matrix as follows:

$$[Q]^m = \begin{Bmatrix} q_i^* \\ q_j^* \\ 0 \end{Bmatrix} \quad . \tag{E-17}$$

Combining the expressions for the surface and line integrals, the following equation in terms of elemental matrices is obtained,

$$[SL]\,\{\psi\}^m + [PL]\,\{\psi_t\}^m + [Q]^m = 0 \tag{E-18}$$

which may be assembled for all the elements in the layout to yield,

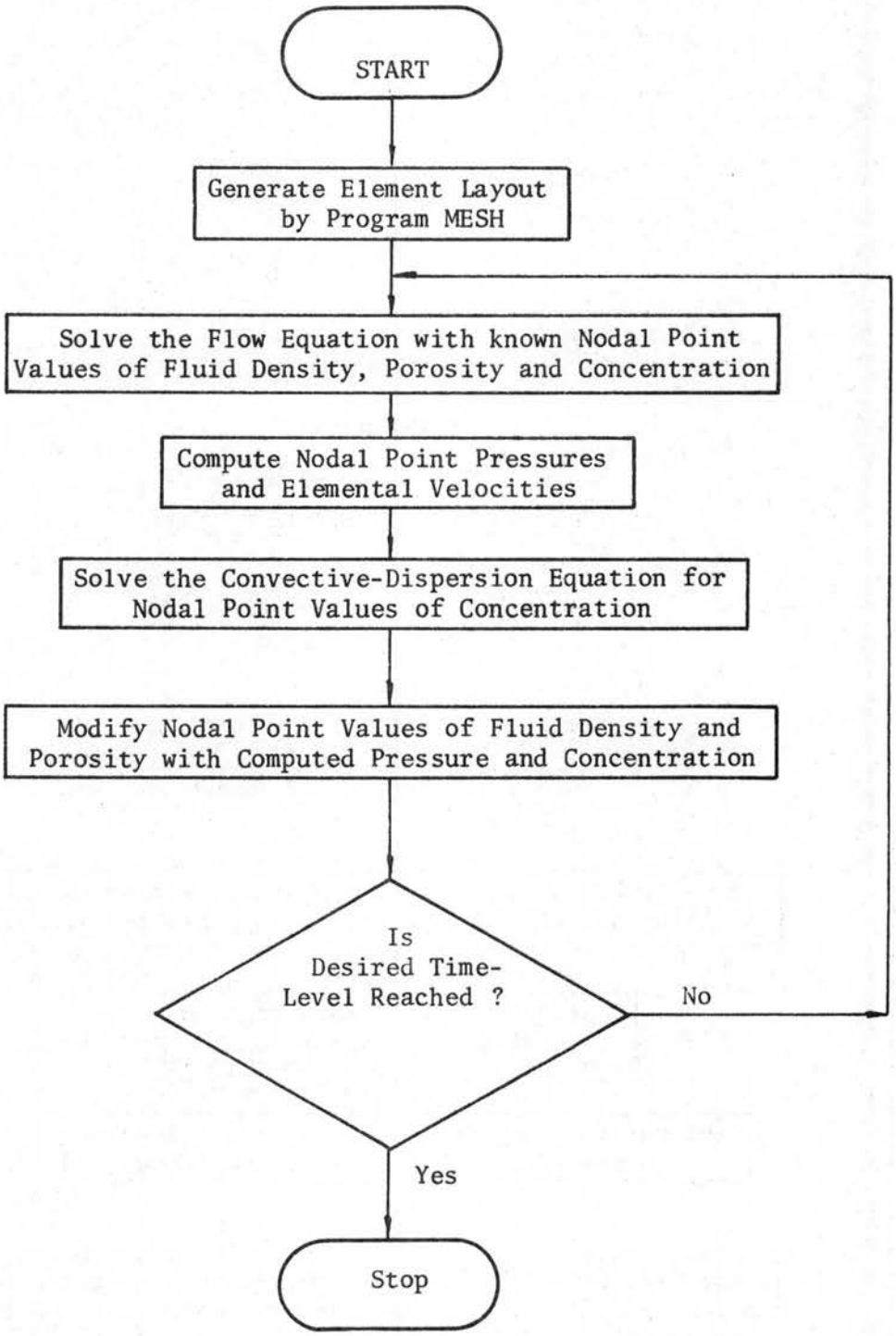
$$[SK]\,\{\psi\} + [PK]\,\{\psi_t\} + [QK] = 0 \tag{E-19}$$

where the assembled matrices [SK] and [PK] are banded and symmetric.

APPENDIX F

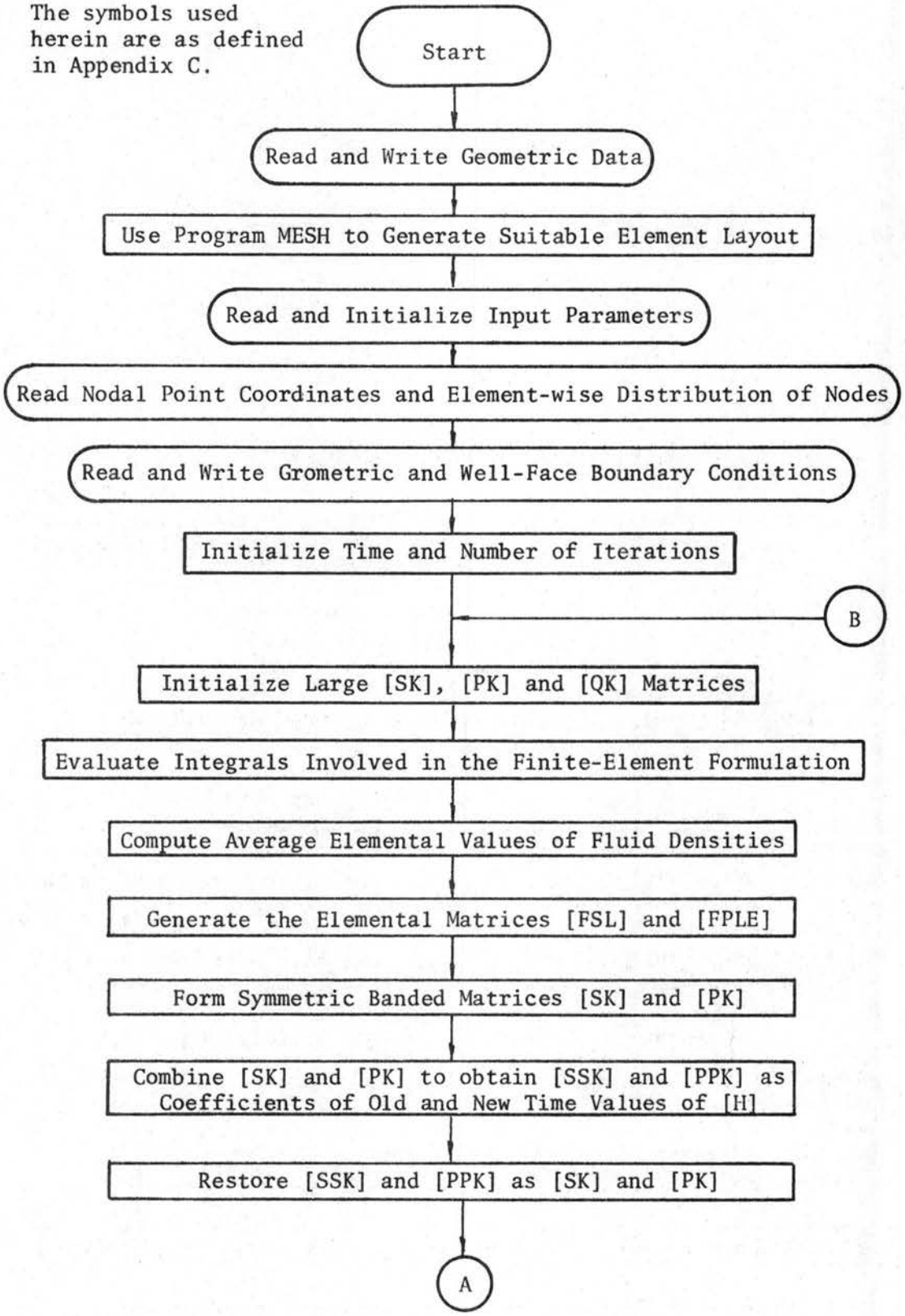
FLOW CHARTS

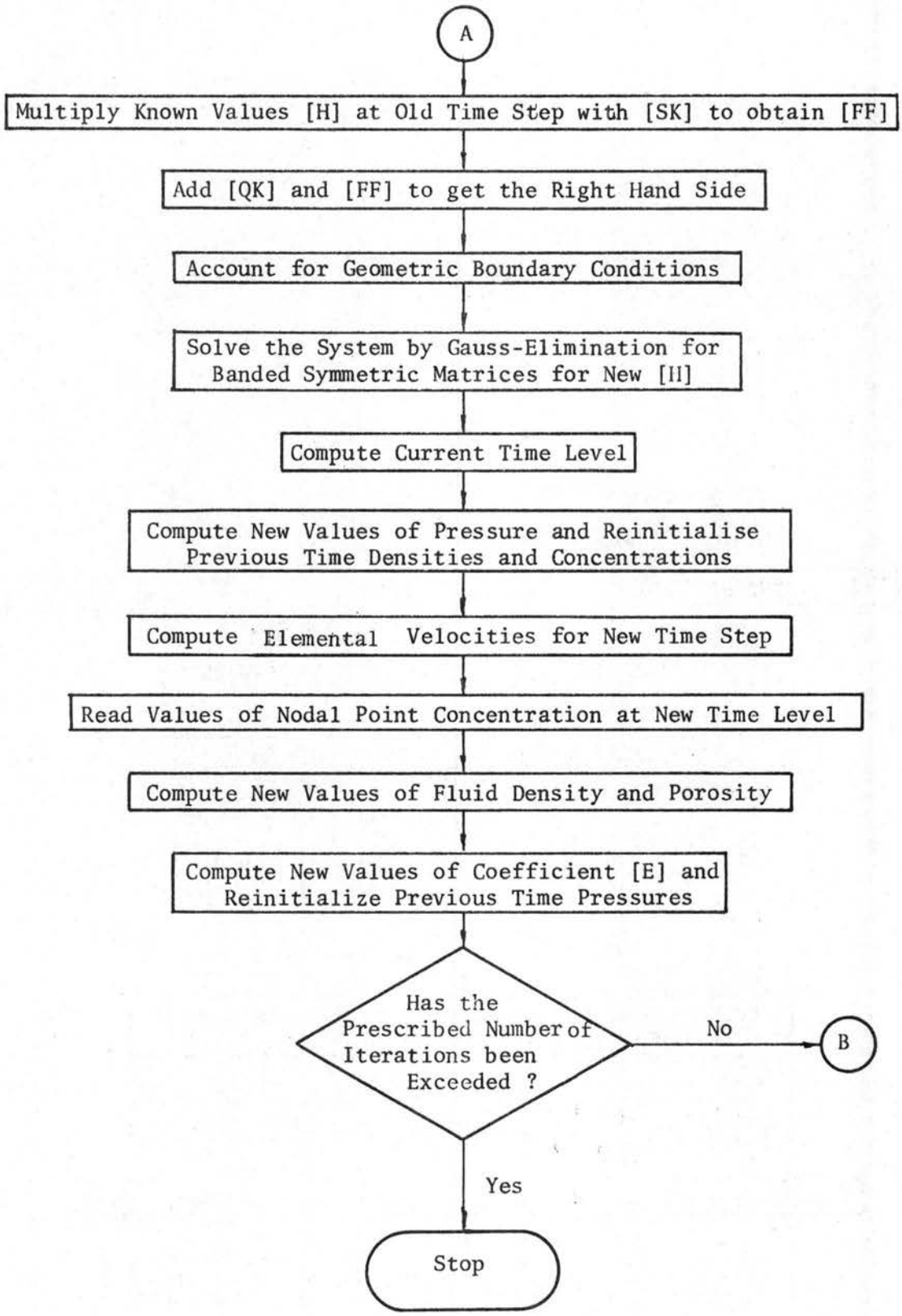
FLOW CHART FOR LEAP-FROG TECHNIQUE



FLOW CHART FOR PROGRAM FLOW

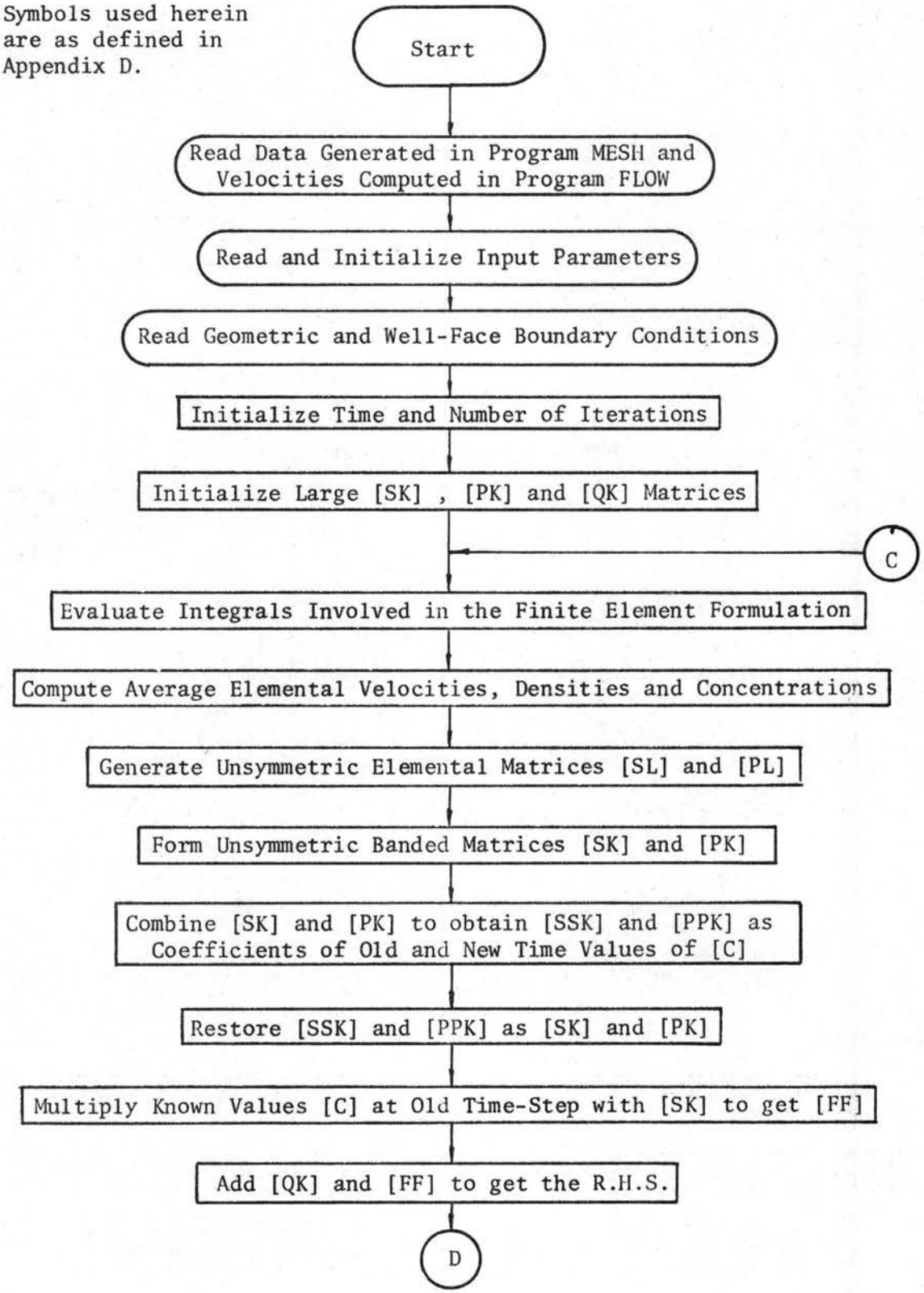
The symbols used herein are as defined in Appendix C.

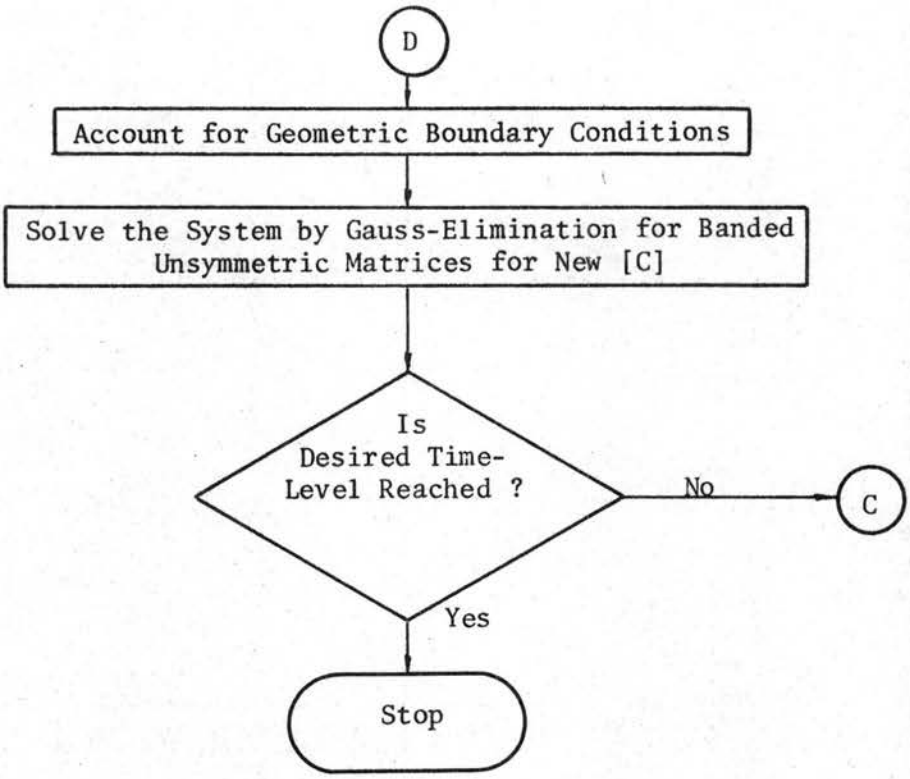



A
Multiply Known Values [H] at Old Time Step with [SK] to obtain [FF]
Add [QK] and [FF] to get the Right Hand Side
Account for Geometric Boundary Conditions
Solve the System by Gauss-Elimination for Banded Symmetric Matrices for New [H]
Compute Current Time Level
Compute New Values of Pressure and Reinitialise Previous Time Densities and Concentrations
Compute Elemental Velocities for New Time Step
Read Values of Nodal Point Concentration at New Time Level
Compute New Values of Fluid Density and Porosity
Compute New Values of Coefficient [E] and Reinitialize Previous Time Pressures
Has the Prescribed Number of Iterations been Exceeded ?
No
B
Yes
Stop

FLOW CHART FOR PROGRAM DISPER

Symbols used herein are as defined in Appendix D.




D
Account for Geometric Boundary Conditions
Solve the System by Gauss-Elimination for Banded Unsymmetric Matrices for New [C]
Is Desired Time-Level Reached ?
No
C
Yes
Stop

APPENDIX G

Program MESH

The data requirements of the program are:

(i) NDIVX = N_x = Number of divisions of the sides along the x-axis.

(ii) NDIVY = N_y = Number of divisions of the sides along the y-axis.

(iii) XMIN = X_1 = Minimum value of x in the layout.

(iv) YMIN = Y_1 = Minimum value of y in the layout.

(v) XMAX = X_3 = Maximum value of x in the layout.

(vi) YMAX = Y_3 = Maximum value of y in the layout.

(vii) Coordinates of eight points a , b , c , d , e , f , g and h on the boundary (Fig. G-1) arranged in a counter-clockwise sense. Say,

[(x_1,y_1), (x_2,y_2),....., (x_7,y_7) and (x_8,y_8)].

With the above data, the program divides the area into N_x x N_y quadrilaterals and joins the shorter diagonal of each to produce a triangular mesh.

For a simple rectangular region, if the boundaries are oriented in such a way that the side with smaller number of divisions is treated as the side along the x-axis, the program generates a mesh with reasonably small band-width. Depending upon the relative positions of the eight boundary points, the sizes of the elements vary in an arithmetic progression as explained below.

Referring to Fig. G-1, if ab < bc , the x-dimension of the elements progressively increases from a to c . Similarly, if ah < gh , the y-dimension increases from a to g . If Ax and Ay are the shortest x and y dimensions of any element and dx and dy are the common differences for the two dimensions, then,

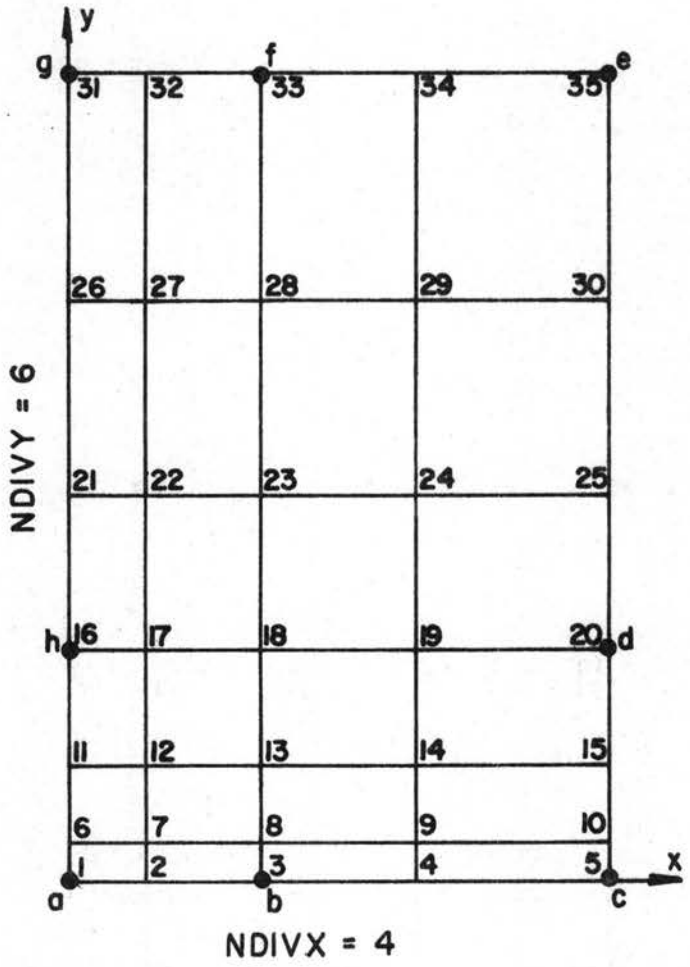


Fig. G.1 Boundary Subdivisions for Program MESH

$$A_x N_x + \frac{N_x - 1}{2} N_x \, dx = X_3 - X_1 \quad . \qquad (G\text{-}1)$$

$$A_x \frac{N_x}{2} + \{ (\frac{N_x}{2} - 1)/2 \} \frac{N_x}{2} \, dx = X_2 - X_1 \quad . \qquad (G\text{-}2)$$

and,

$$A_y N_y + \frac{N_y - 1}{2} \, dy \, N_y = Y_3 - Y_1 \quad , \qquad (G\text{-}3)$$

$$A_y \frac{N_y}{2} + \{ (\frac{N_y}{2} - 1)/2 \} \, dy \, \frac{N_y}{2} = Y_3 - Y_1 \quad . \qquad (G\text{-}4)$$

Therefore,

$$dx = 4 \, (X_3 - 2X_2 + X_1)/N_x^2 \qquad (G\text{-}5)$$

$$dy = 4 \, (2Y_2 - Y_3 - Y_1)/N_y^2 \quad . \qquad (G\text{-}6)$$

Knowing dx and dy , A_x and A_y may be calculated, the x and y dimensions of the elements proceeding from a to c and from a to g respectively will be,

A_x, A_x+dx, A_x+2dx,....., A_x+(N_x-1) dx and

A_y, A_y+dy, A_y+2dy,....., A_y+(N_y-1) dy .

Theoretically, any sizes of A_x and A_y (as small as required) can be accomodated provided that there is no limitation to the numbers N_x and N_y for a given size of the region.

For complex regions, the area is divided into two or more loops for providing different sizes of elements in different portions as shown in Fig. 4.1. The above algorithm is then applied to each loop in succession.

Additional data required for this case are:

(i) NUMLPS = Number of loops, and

(ii) JOIN(I,J,K) array, which for the loops shown in Fig. 4.1 is defined in the following table.

TABLE G-1

JOIN(I,J,K) ARRAY

Loop (I) ↓	k=1 Loop No.	k=2 Side No.	k=1 Loop No.	k=2 Side No.	k=1 Loop No.	k=2 Side No.	k=1 Loop No.	k=2 Side No.
1	0	0	0	0	0	0	0	0
2	1	3	0	0	0	0	0	0
3	1	2	0	0	0	0	2	2
Side (J) →	1		2		3		4	

The above table is read as follows:

Side (J) of loop (I) is common with the side given under column k=2 of the loop number given under column k=1 . This interconnection is referred only backwards with respect to the loop numbers. Thus sides of loop 1 are entered in the above table as not common (denoted by 0) with those of loops 2 and 3, and sides of loop 2 are entered as common with the sides of loop 1 but not common with those of loop 3.

For multi-loop regions, the above procedure results in a very large band-width. Therefore, two subroutines have been introduced in this program for band-width reduction. The first of these subroutines arranges the data in a form suitable for the application of the second subroutine. The latter subroutine renumbers all the nodes in the system so as to yield a minimum band-width. A listing of this program is given in Appendix H.

APPENDIX H

PROGRAM LISTINGS

PROGRAM FFLOW

```
      PROGRAM FFLOW (INPUT=101R,PUNCH,OUTPUT=202R,TAPE5=INPUT,TAPE6=OUTP      A   10
     1UT,TAPE8=PUNCH)                                                         A   20
      COMMON /RLK3/ SK(300,20)                                                A   30
      COMMON /RLK4/ PK(300,20)                                                A   40
      COMMON /RLK5/ QK(300)                                                   A   50
      COMMON /RLK6/ NP(450,3),P(300),Z(300)                                   A   60
      COMMON /RLK7/ PHI0(300)                                                 A   70
      COMMON /RLK8/ VR(450),VZ(450),FK(450),RHO(300),C(300)                   A   80
      DIMENSION RLOC(3), ZLOC(3), FPLE(3,3), FSL(3,3), H(300), NPBC(300)      A   90
     1, HBC(300), PP(300), AP(300), AC(300), E(300), RHOO(300), PPK(300,      A  100
     225), SSK(300,25), FF(300), KP(450,3), LP(450,3), PL(3,3), SL(3,3),      A  110
     3 CBC(300)                                                               A  120
      DATA NUMNP,NUMEL,IBAND,NUMBC,ALPHA,ABETA,CF,DT,AMU,ITT,PENETR,DIV,      A  130
     1FQ,NBCWL,RW,AL,ATL,DD,T,GG,PI/200,312,7,5,.74,2.3E-8,.6E-8,.1,2.4F      A  140
     2-5,500,100,.4,.1,.5,.5,.1,0,.0,.5,32.2,3.1415926/                       A  150
C                                                                             A  160
C     THIS PROGRAM SOLVES FLOW AND CONVECTIVE-DISPERSION EQUATIONS IN         A  170
C     RADIAL COORDINATES.                                                     A  180
C     NUMNP=NO. OF NODAL POINTS                                               A  190
C     NUMEL=NO. OF ELEMENTS                                                   A  200
C     NP(I,J)=ARRAY GIVING ASSIGNED NO. TO JTH NODE OF ELEMENT NO. I          A  210
C     VR(I)=VELOCITY COMPONENT OF ELEMENT NO. I IN R-DIRECTION                A  220
C     VZ(I)=VELOCITY COMPONENT OF ELEMENT NO. I IN Z-DIRECTION                A  230
C     NPBC(N)=0 SIGNIFIES THAT NO B.C. IS SPECIFIED AT NODE NO. N             A  240
C     NPBC(N)=1 SIGNIFIES THAT B.C. IS GIVEN AT NODE NO. N                    A  250
C     NPBC(N)=2 SIGNIFIES WELL BOUNDARY                                       A  260
C     NUMBC= NUMBER OF NODES AT WHICH B.C. IS GIVEN                           A  270
C     NBCWL=NUMBER OF NODAL POINTS ON THE WELL FACE                           A  280
C     RW=RADIUS OF WELL                                                       A  290
C     PHI0=INITIAL POROSITY                                                   A  300
C     AMU=DYNAMIC VISCOSITY                                                   A  310
C     AL=LONGITUDINAL DISPERSIVITY                                            A  320
C     ATL=TRANSVERSE DISPERSIVITY                                             A  330
C     DD=COEFF. OF MOLECULAR DIFFUSION                                        A  340
C     T=TORTUOSITY                                                            A  350
C     DIV=NO. OF DIVISIONS OF PENETRATION DEPTH                               A  360
C     PENETR=DEPTH OF WELL PENETRATION                                        A  370
C     DT=TIME INCREMENT.                                                      A  380
C     CF=AQUIFER COMPRESSIBILITY                                              A  390
C     ABETA=FLUID COMPRESSIBILITY                                             A  400
C     ALPHA=FACTOR RELATING RHO WITH C                                        A  410
C     FQ=WELL DISCHARGE                                                       A  420
C     FK=INTRINSIC PERMEABILITY                                               A  430
C     RHOO=INITIAL FLUID DENSITY                                              A  440
C     AP=VALUE OF P AT PREVIOUS TIME                                          A  450
C     P=CURRENT VALUE OF PRESSURE                                             A  460
C     ITT=NO. OF TIME PERIODS OVER WHICH SOLUTION IS REQUIRED                 A  470
C                                                                             A  480
C                                                                             A  490
C     READ AND INITIALISE DATA                                                A  500
      READ (5,144) (FK(I),I=1,NUMEL)                                          A  510
      READ (5,144) (PHO(I),I=1,NUMNP)                                         A  520
      READ (5,144) (PHI0(I),I=1,NUMNP)                                        A  530
      READ (5,144) (H(I),I=1,NUMNP)                                           A  540
      READ (5,144) (C(I),I=1,NUMNP)                                           A  550
      READ (5,147) (N,Z(N),Q(N),NN=1,NUMNP)                                   A  560
      READ (5,146) (K,KP(K,1),KP(K,2),KP(K,3),KK=1,NUMEL)                    A  570
      READ (5,146) (L,LP(L,1),LP(L,2),LP(L,3),LL=1,NUMEL)                    A  580
C                                                                             A  590
      DZ=PENETR/DIV                                                           A  600
      DFQ=-(FQ*DZ)/(4.0*PI*PENETR)                                            A  610
      M=IBAND                                                                 A  620
      KBAND=(2*M)-1                                                           A  630
      DO 101 I=1,NUMNP                                                        A  640
         HBC(I)=0.0                                                           A  650
         NPBC(I)=0                                                            A  660
         RHOO(I)=RHO(I)                                                       A  670
         CBC(I)=0.0                                                           A  680
  101 CONTINUE                                                                A  690
C                                                                             A  700
C     READ AND WRITE BOUNDARY CONDITIONS                                      A  710
C                                                                             A  720
      READ (5,143) (N,NPBC(N),HBC(N),CBC(N),NN=1,NUMBC)                       A  730
      READ (5,150) (N,NPBC(N),NN=1,NBCWL)                                     A  740
C                                                                             A  750
      DO 102 I=1,NUMNP                                                        A  760
         IF (NPBC(I).EQ.1) H(I)=HBC(I)                                        A  770
         F(I)=RHOO(I)*PHI0(I)*(ABETA+CF)                                      A  780
         AP(I)=H(I)-(RHOO(I)*GG*Z(I))                                         A  790
  102 CONTINUE                                                                A  800
      TIME=0.0                                                                A  810
      KT=0                                                                    A  820
      INT=10                                                                  A  830
      INTR=10                                                                 A  840
  103 KT=KT+1                                                                 A  850
      JK=1                                                                    A  860
  104 CONTINUE                                                                A  870
      JL=0                                                                    A  880
  105 CONTINUE                                                                A  890
      JL=JL+1                                                                 A  900
      IF (JL-1) 109,106,109                                                   A  910
  106 CONTINUE                                                                A  920
      DO 108 N=1,NUMEL                                                        A  930
         DO 107 J=1,3                                                         A  940
            NP(N,J)=KP(N,J)                                                   A  950
  107    CONTINUE                                                            A  960
  108 CONTINUE                                                                A  970
      GO TO 112                                                               A  980
  109 CONTINUE                                                                A  990
      DO 111 N=1,NUMEL                                                        A 1000
         DO 110 J=1,3                                                         A 1010
            NP(N,J)=LP(N,J)                                                   A 1020
  110    CONTINUE                                                            A 1030
  111 CONTINUE                                                                A 1040
  112 CONTINUE                                                                A 1050
      DO 114 I=1,NUMNP                                                        A 1060
         IF (NPBC(I).EQ.1) C(I)=CBC(I)                                        A 1070
         IF (NPBC(I).EQ.1) H(I)=HBC(I)                                        A 1080
         QK(I)=0.0                                                            A 1090
         DO 113 J=1,IBAND                                                     A 1100
            SK(I,J)=0.0                                                       A 1110
            PK(I,J)=0.0                                                       A 1120
  113    CONTINUE                                                            A 1130
  114 CONTINUE                                                                A 1140
C                                                                             A 1150
C                                                                             A 1160
      DO 116 I=1,NUMEL                                                        A 1170
         CALL CENTOD (I,RBAR,ZBAR)                                            A 1180
         CALL CLOCAL (I,RBAR,ZBAR,RLOC,ZLOC)                                  A 1190
         CALL AREA (RLOC,ZLOC,AM)                                             A 1200
         CALL TEGRAL (RLOC,ZLOC,AM,FXXET,FXXX,FXETT,XISQ,TASQ,XITA)           A 1210
         CALL PHOSEL (I,PHOEL,PHOOFL,RHOO,RHO)                                A 1220
         IF (JK.NE.1) GO TO 115                                               A 1230
         S=RHOEL*FK(I)/AMU                                                    A 1240
         CALL FSLPL (RLOC,ZLOC,RBAR,AM,FXXET,FXETT,FXXX,XISQ,XITA,TASQ,F      A 1250
        1   SL,FPLE,S)                                                        A 1260
         CALL FSLSK (FSL,FPLE,I,DFQ,NPBC,RHO)                                 A 1270
         GO TO 116                                                            A 1280
  115    CONTINUE                                                            A 1290
```

```
      CALL FLVFL (I,RLOC,ZLOC,M,AMU,AM)                                  A 1300
      CALL SLPL (RLOC,ZLOC,PBAR,AM,PL,SL,ALPHA,AL,DD,T,All,EXXFT,FXXX    A 1310
     1   ,EXFTT,RHOEL,XISO,TASO,XITA,I)                                  A 1320
      CALL SLSK (SL,PL,DFQ,T,NPRC,C,IRAND)                               A 1330
  116 CONTINUE                                                           A 1340
C                                                                        A 1350
      IF (JL.GT.1) GO TO 119                                             A 1360
C                                                                        A 1370
      DO 118 I=1,NUMNP                                                   A 1380
         DO 117 J=1,IRAND                                                A 1390
            PPK(I,J)=PK(I,J)                                             A 1400
            SSK(I,J)=SK(I,J)                                             A 1410
  117    CONTINUE                                                        A 1420
  118 CONTINUE                                                           A 1430
      GO TO 105                                                          A 1440
  119 CONTINUE                                                           A 1450
      DO 121 I=1,NUMNP                                                   A 1460
         DO 120 J=1,IRAND                                                A 1470
            SK(I,J)=(SSK(I,J)+SK(I,J))/2.                                A 1480
            PK(I,J)=(PPK(I,J)+PK(I,J))/2.                                A 1490
  120    CONTINUE                                                        A 1500
  121 CONTINUE                                                           A 1510
      IF (JK.NE.1) GO TO 124                                             A 1520
      DO 123 I=1,NUMNP                                                   A 1530
         DO 122 J=1,IRAND                                                A 1540
            PPK(I,J)=(SK(I,J)/2.0)+(E(I)*PK(I,J)/DT)                     A 1550
            SSK(I,J)=((F(I)*PK(I,J)/DT)-(SK(I,J)/2.0))                   A 1560
  122    CONTINUE                                                        A 1570
  123 CONTINUE                                                           A 1580
      GO TO 127                                                          A 1590
  124 CONTINUE                                                           A 1600
      DO 126 I=1,NUMNP                                                   A 1610
         DO 125 J=1,IRAND                                                A 1620
            PPK(I,J)=(SK(I,J)/2.0)+(PK(I,J)/DT)                          A 1630
            SSK(I,J)=(PK(I,J)/DT)-(SK(I,J)/2.0)                          A 1640
  125    CONTINUE                                                        A 1650
  126 CONTINUE                                                           A 1660
  127 CONTINUE                                                           A 1670
      DO 129 I=1,NUMNP                                                   A 1680
         DO 128 J=1,IRAND                                                A 1690
            PK(I,J)=PPK(I,J)                                             A 1700
            SK(I,J)=SSK(I,J)                                             A 1710
  128    CONTINUE                                                        A 1720
  129 CONTINUE                                                           A 1730
      IF (JK.NE.1) GO TO 133                                             A 1740
      CALL FSKPSI (H,NUMNP,IRAND,FF)                                     A 1750
      DO 131 I=1,NUMNP                                                   A 1760
         FF(I)=QK(I)+FF(I)                                               A 1770
C                                                                        A 1780
C     ACCOUNT FOR BOUNDARY CONDITIONS                                    A 1790
C                                                                        A 1800
         IF (NPRC(I)-1) 131,130,131                                      A 1810
  130    PK(I,1)=PK(I,1)*1.0E+50                                         A 1820
         FF(I)=PRC(I)*PK(I,1)                                            A 1830
  131 CONTINUE                                                           A 1840
      CALL GAUSS (NUMNP,IRAND,FF)                                        A 1850
      DO 132 I=1,NUMNP                                                   A 1860
         H(I)=FF(I)                                                      A 1870
         PP(I)=H(I)-(RHO(I)*GG*Z(I))                                     A 1880
         RHOO(I)=RHO(I)                                                  A 1890
         AC(I)=C(I)                                                      A 1900
  132 CONTINUE                                                           A 1910
C                                                                        A 1920
      IF (KT.NE.INT) GO TO 137                                           A 1930
      JK=JK+1                                                            A 1940
      IRAND=KRAND                                                        A 1950
      GO TO 104                                                          A 1960
  133 CONTINUE                                                           A 1970
      CALL SKPSI (C,NUMNP,IRAND,FF)                                      A 1980
      DO 135 I=1,NUMNP                                                   A 1990
         FF(I)=-QK(I)+FF(I)                                              A 2000
C                                                                        A 2010
C     ACCOUNT FOR BOUNDARY CONDITIONS                                    A 2020
C                                                                        A 2030
         IF (NPRC(I)-1) 135,134,135                                      A 2040
  134    PK(I,M)=PK(I,M)*1.0E+50                                         A 2050
         FF(I)=PRC(I)*PK(I,M)                                            A 2060
  135 CONTINUE                                                           A 2070
      CALL BSOLVE (NUMNP,IBAND,FF)                                       A 2080
      DO 136 I=1,NUMNP                                                   A 2090
      C(I)=FF(I)                                                         A 2100
  136 CONTINUE                                                           A 2110
  137 CONTINUE                                                           A 2120
      DO 138 I=1,NUMNP                                                   A 2130
         RHO(I)=RHOO(I)+(ARETA*RHOO(I)*(PP(I)-AP(I)))+(ALPHA*(C(I)-AC(I) A 2140
     1   ))                                                              A 2150
         PHIO(I)=PHIO(I)*(1.+CF*(PP(I)-AP(I)))                           A 2160
  138 CONTINUE                                                           A 2170
      DO 139 I=1,NUMNP                                                   A 2180
         F(I)=PHOO(I)*PHIO(I)*(ARETA+CF)                                 A 2190
         AP(I)=PP(I)                                                     A 2200
  139 CONTINUE                                                           A 2210
      TIME=TIME+DT                                                       A 2220
      IF (KT.NE.INT) GO TO 141                                           A 2230
      INT=INT+INTP                                                       A 2240
      IRAND=M                                                            A 2250
      WRITE (6,145) KT,TIME,DT                                           A 2260
      WRITE (6,148)                                                      A 2270
      WRITE (6,142) (H(I),I=1,NUMNP)                                     A 2280
      WRITE (6,149)                                                      A 2290
      WRITE (6,142) (C(I),I=1,NUMNP)                                     A 2300
C                                                                        A 2310
      CALL SECOND (B)                                                    A 2320
      A=SECOND(B)                                                        A 2330
      IF (A.LT.600.) GO TO 141                                           A 2340
      WRITE (8,144) (H(I),I=1,NUMNP)                                     A 2350
      WRITE (8,144) (C(I),I=1,NUMNP)                                     A 2360
  141 CONTINUE                                                           A 2370
      IF (KT.LT.10) GO TO 103                                            A 2380
      DT=1.                                                              A 2390
      IF (KT.LT.20) GO TO 103                                            A 2400
      DT=10.0                                                            A 2410
      IF (KT.LT.30) GO TO 103                                            A 2420
      DT=100.0                                                           A 2430
      IF (KT.LT.40) GO TO 103                                            A 2440
      DT=1000.                                                           A 2450
      IF (KT.LT.50) GO TO 103                                            A 2460
      DT=10000.                                                          A 2470
      IF (KT.LT.60) GO TO 103                                            A 2480
      DT=100000.                                                         A 2490
      IF (KT.LT.70) GO TO 103                                            A 2500
      DT=1000000.                                                        A 2510
      IF (KT.LT.ITT) GO TO 103                                           A 2520
      STOP                                                               A 2530
C                                                                        A 2540
  142 FORMAT (5E18.8)                                                    A 2550
  143 FORMAT (2I10,2F16.8)                                               A 2560
  144 FORMAT (5E14.8)                                                    A 2570
  145 FORMAT (/I20,2F20.3/)                                              A 2580
  146 FORMAT (4I10)                                                      A 2590
  147 FORMAT (I10,2F10.2)                                                A 2600
  148 FORMAT (/, 52H                          VALUES OF H                A 2610
     1,/)                                                                A 2620
  149 FORMAT (/, 56H                       VALUES OF CONCENTRA            A 2630
```

```
     1TION,/)                                                          A 2640
  150 FORMAT (2I10)                                                    A 2650
C                                                                      A 2660
      END                                                              A 2670
```

SUBROUTINE CENTOD

```
      SUBROUTINE CENTOD (M,RBAR,ZBAR)                                  B   10
C                                                                      B   20
C     THIS SUBROUTINE COMPUTES COORDINATES OF THE CENTROID OF THE TRIANG B   30
C     ULAR ELEMENT NO. M                                               B   40
C                                                                      B   50
      COMMON /RLK6/ NP(450,3),R(300),Z(300)                            B   60
      I=NP(M,1)                                                        B   70
      J=NP(M,2)                                                        B   80
      K=NP(M,3)                                                        B   90
      RBAR=(R(I)+R(J)+R(K))/3.                                         B  100
      ZBAR=(Z(I)+Z(J)+Z(K))/3.                                         B  110
      RETURN                                                           B  120
C                                                                      B  130
      END                                                              B  140
```

SUBROUTINE CLOCAL

```
      SUBROUTINE CLOCAL (M,RBAR,ZBAR,RLOC,ZLOC)                        C   10
C                                                                      C   20
C     THIS SUBROUTINE COMPUTES LOCAL COORDINATES OF THE NODES OF THE TRI C   30
C     ANGULAR ELEMENT NO. M                                            C   40
C                                                                      C   50
      COMMON /RLK6/ NP(450,3),R(300),Z(300)                            C   60
      DIMENSION RLOC(3), ZLOC(3)                                       C   70
      DO 101 L=1,3                                                     C   80
         I=NP(M,L)                                                     C   90
         RLOC(L)=R(I)-RBAR                                             C  100
  101 ZLOC(L)=Z(I)-ZBAR                                                C  110
      RETURN                                                           C  120
C                                                                      C  130
      END                                                              C  140
```

SUBROUTINE AREA

```
      SUBROUTINE AREA (RLOC,ZLOC,AM)                                   D   10
C                                                                      D   20
C     THIS SUBROUTINE CALCULATES AREA OF THE TRIANGULAR ELEMENT NO. M  D   30
C                                                                      D   40
      DIMENSION RLOC(3), ZLOC(3)                                       D   50
      AM=(RLOC(2)*ZLOC(3)-RLOC(3)*ZLOC(2)-RLOC(1)*ZLOC(3)+RLOC(3)*ZLOC(1 D   60
     1)+RLOC(1)*ZLOC(2)-RLOC(2)*ZLOC(1))/2.                            D   70
      RETURN                                                           D   80
C                                                                      D   90
      END                                                              D  100
```

SUBROUTINE TEGRAL

```
      SUBROUTINE TEGRAL (RLOC,ZLOC,AM,EXXET,FXXX,EXETT,XISQ,TASQ,XITA) E   10
      COMMON /RLK6/ NP(450,3),R(300),Z(300)                            E   20
      DIMENSION RLOC(3), ZLOC(3), AJ(3), H(3), AI(3), AS(3)            E   30
      AAM=ABS(AM)                                                      E   40
      AJ(1)=.1127016654                                                E   50
      AJ(2)=.5                                                         E   60
      AJ(3)=.8872983346                                                E   70
      H(1)=.2777777779                                                 E   80
      H(2)=.4444444444                                                 E   90
      H(3)=H(1)                                                        E  100
      AI(1)=.0885879595                                                E  110
      AI(2)=.4094668644                                                E  120
      AI(3)=.7876594618                                                E  130
      AS(1)=.2204622112                                                E  140
      AS(2)=.3881934688                                                F  150
      AS(3)=.3288443200                                                F  160
      XITA=0.                                                          E  170
      XISQ=0.                                                          F  180
      TASQ=0.                                                          E  190
      EXXET=0.                                                         E  200
      EXXX=0.                                                          E  210
      EXETT=0.                                                         E  220
      DO 102 I=1,3                                                     E  230
         RL1=AI(I)                                                     E  240
         DO 101 J=1,3                                                  E  250
            RL2=AJ(J)*(1.-RL1)                                         E  260
            RL3=1.-RL1-RL2                                             E  270
            W=AS(I)*H(J)*(1.-RL1)*2.*AAM                               F  280
            X=RL1*RLOC(1)+RL2*RLOC(2)+RL3*RLOC(3)                      E  290
            Y=RL1*ZLOC(1)+RL2*ZLOC(2)+RL3*ZLOC(3)                      E  300
            XITA=XITA+X*Y*W                                            E  310
            XISQ=XISQ+X*X*W                                            E  320
            TASQ=TASQ+Y*Y*W                                            E  330
            EXXET=FXXT+X*X*Y*W                                         E  340
            EXXX=FXXX+X*X*X*W                                          E  350
            EXETT=EXETT+X*Y*Y*W                                        E  360
  101    CONTINUE                                                      F  370
  102 CONTINUE                                                         E  380
      RETURN                                                           E  390
C                                                                      F  400
      END                                                              F  410
```

SUBROUTINE FSLPL

```
      SUBROUTINE FSLPL (RLOC,ZLOC,RBAR,AM,EXXET,EXETT,FXXX,XISQ,XITA,TAS F   10
     1Q,FSL,FPLF,S)                                                    F   20
C                                                                      F   30
C     THIS SUBROUTINE COMPUTES THE FSL,FPLF,FRHO, AND FPLF MATRICES    F   40
C                                                                      F   50
      DIMENSION RLOC(3), ZLOC(3), SAA(3,3), SALPHA(3,3), SBETA(3,3), SGA F   60
     1MA(3,3), STHETA(3,3), SA(3,3), SC(3,3), FPLF(3,3), FSL(3,3)      F   70
      XII=RLOC(1)                                                      F   80
      XIJ=RLOC(2)                                                      F   90
      XIK=RLOC(3)                                                      F  100
      TAI=ZLOC(1)                                                      F  110
      TAJ=ZLOC(2)                                                      F  120
      TAK=ZLOC(3)                                                      F  130
      A1I=XIJ*TAK-TAJ*XIK                                              F  140
```

```
      A2I=TAJ-TAK                                                       F  150
      A3I=XIK-XIJ                                                       F  160
      A1J=XIK*TAI-TAK*XII                                               F  170
      A2J=TAK-TAI                                                       F  180
      A3J=XII-XIK                                                       F  190
      A1K=XII*TAJ-TAI*XIJ                                               F  200
      A2K=TAI-TAJ                                                       F  210
      A3K=XIJ-XII                                                       F  220
      AAM=ABS(AM)                                                       F  230
C                                                                       F  240
C     COMPUTE ELEMENTS OF SA MATRIX                                     F  250
C                                                                       F  260
      COFSA=(RBAR*S*AAM)/(4.0*AM*AM)                                    F  270
      SA(1,1)=COFSA*A2I*A2I                                             F  280
      SA(1,2)=COFSA*A2I*A2J                                             F  290
      SA(1,3)=COFSA*A2I*A2K                                             F  300
      SA(2,1)=COFSA*A2J*A2I                                             F  310
      SA(2,2)=COFSA*A2J*A2J                                             F  320
      SA(2,3)=COFSA*A2J*A2K                                             F  330
      SA(3,1)=COFSA*A2K*A2I                                             F  340
      SA(3,2)=COFSA*A2K*A2J                                             F  350
      SA(3,3)=COFSA*A2K*A2K                                             F  360
C                                                                       F  370
C     COMPUTE ELEMENTS OF SC MATRIX                                     F  380
C                                                                       F  390
      COFSC=COFSA                                                       F  400
      SC(1,1)=COFSC*A3I*A3I                                             F  410
      SC(1,2)=COFSC*A3I*A3J                                             F  420
      SC(1,3)=COFSC*A3I*A3K                                             F  430
      SC(2,1)=COFSC*A3J*A3I                                             F  440
      SC(2,2)=COFSC*A3J*A3J                                             F  450
      SC(2,3)=COFSC*A3J*A3K                                             F  460
      SC(3,1)=COFSC*A3K*A3I                                             F  470
      SC(3,2)=COFSC*A3K*A3J                                             F  480
      SC(3,3)=COFSC*A3K*A3K                                             F  490
C                                                                       F  500
C     COMPUTE ELEMENTS OF SAA MATRIX                                    F  510
C                                                                       F  520
      CSAA=AAM                                                          F  530
      COFSAA=RBAR/(4.0*AM*AM)                                           F  540
      SAA(1,1)=(CSAA*A1I*A1I+A2I*A2I*XISQ+(A2I*A3I+A3I*A2I)*XITA+A3I*A3I F  550
     1*TASQ)*COFSAA                                                     F  560
      SAA(1,2)=(CSAA*A1J*A1I+A2J*A2I*XISQ+(A2J*A3I+A3J*A2I)*XITA+A3J*A3I F  570
     1*TASQ)*COFSAA                                                     F  580
      SAA(1,3)=(CSAA*A1K*A1I+A2K*A2I*XISQ+(A2K*A3I+A3K*A2I)*XITA+A3K*A3I F  590
     1*TASQ)*COFSAA                                                     F  600
      SAA(2,1)=(CSAA*A1I*A1J+A2I*A2J*XISQ+(A2I*A3J+A3I*A2J)*XITA+A3I*A3J F  610
     1*TASQ)*COFSAA                                                     F  620
      SAA(2,2)=(CSAA*A1J*A1J+A2J*A2J*XISQ+(A2J*A3J+A3J*A2J)*XITA+A3J*A3J F  630
     1*TASQ)*COFSAA                                                     F  640
      SAA(2,3)=(CSAA*A1K*A1J+A2K*A2J*XISQ+(A2K*A3J+A3K*A2J)*XITA+A3K*A3J F  650
     1*TASQ)*COFSAA                                                     F  660
      SAA(3,1)=(CSAA*A1I*A1K+A2I*A2K*XISQ+(A2I*A3K+A3I*A2K)*XITA+A3I*A3K F  670
     1*TASQ)*COFSAA                                                     F  680
      SAA(3,2)=(CSAA*A1J*A1K+A2J*A2K*XISQ+(A2J*A3K+A3J*A2K)*XITA+A3J*A3K F  690
     1*TASQ)*COFSAA                                                     F  700
      SAA(3,3)=(CSAA*A1K*A1K+A2K*A2K*XISQ+(A2K*A3K+A3K*A2K)*XITA+A3K*A3K F  710
     1*TASQ)*COFSAA                                                     F  720
C                                                                       F  730
C     COMPUTE ELEMENTS OF SALPHA MATRIX                                 F  740
C                                                                       F  750
      SALPHA(1,1)=(A2I*A1I+A1I*A2I)*XISQ+(A3I*A1I+A1I*A3I)*XITA         F  760
      SALPHA(1,2)=(A2I*A1J+A1I*A2J)*XISQ+(A3I*A1J+A1I*A3J)*XITA         F  770
      SALPHA(1,3)=(A2I*A1K+A1I*A2K)*XISQ+(A3I*A1K+A1I*A3K)*XITA         F  780
      SALPHA(2,1)=(A2J*A1I+A1J*A2I)*XISQ+(A3J*A1I+A1J*A3I)*XITA         F  790
      SALPHA(2,2)=(A2J*A1J+A1J*A2J)*XISQ+(A3J*A1J+A1J*A3J)*XITA         F  800
      SALPHA(2,3)=(A2J*A1K+A1J*A2K)*XISQ+(A3J*A1K+A1J*A3K)*XITA         F  810
      SALPHA(3,1)=(A2K*A1I+A1K*A2I)*XISQ+(A3K*A1I+A1K*A3I)*XITA         F  820
      SALPHA(3,2)=(A2K*A1J+A1K*A2J)*XISQ+(A3K*A1J+A1K*A3J)*XITA         F  830
      SALPHA(3,3)=(A2K*A1K+A1K*A2K)*XISQ+(A3K*A1K+A1K*A3K)*XITA         F  840
      DO 102 I=1,3                                                      F  850
         DO 101 J=1,3                                                   F  860
            SALPHA(I,J)=SALPHA(I,J)/(4.0*AM*AM)                         F  870
  101    CONTINUE                                                       F  880
  102 CONTINUE                                                          F  890
C                                                                       F  900
C     COMPUTE ELEMENTS OF SBETA MATRIX                                  F  910
C                                                                       F  920
      COFBTA=EXXET/(4.*AM*AM)                                           F  930
      SBETA(1,1)=COFBTA*(A2I*A3I+A3I*A2I)                               F  940
      SBETA(1,2)=COFBTA*(A2I*A3J+A3I*A2J)                               F  950
      SBETA(1,3)=COFBTA*(A2I*A3K+A3I*A2K)                               F  960
      SBETA(2,1)=COFBTA*(A2J*A3I+A3J*A2I)                               F  970
      SBETA(2,2)=COFBTA*(A2J*A3J+A3J*A2J)                               F  980
      SBETA(2,3)=COFBTA*(A2J*A3K+A3J*A2K)                               F  990
      SBETA(3,1)=COFBTA*(A2K*A3I+A3K*A2I)                               F 1000
      SBETA(3,2)=COFBTA*(A2K*A3J+A3K*A2J)                               F 1010
      SBETA(3,3)=COFBTA*(A2K*A3K+A3K*A2K)                               F 1020
C                                                                       F 1030
C     COMPUTE ELEMENTS OF SGAMA MATRIX                                  F 1040
C                                                                       F 1050
      COFGMA=EXXX/(4.*AM*AM)                                            F 1060
      SGAMA(1,1)=COFGMA*A2I*A2I                                         F 1070
      SGAMA(1,2)=COFGMA*A2I*A2J                                         F 1080
      SGAMA(1,3)=COFGMA*A2I*A2K                                         F 1090
      SGAMA(2,1)=COFGMA*A2J*A2I                                         F 1100
      SGAMA(2,2)=COFGMA*A2J*A2J                                         F 1110
      SGAMA(2,3)=COFGMA*A2J*A2K                                         F 1120
      SGAMA(3,1)=COFGMA*A2K*A2I                                         F 1130
      SGAMA(3,2)=COFGMA*A2K*A2J                                         F 1140
      SGAMA(3,3)=COFGMA*A2K*A2K                                         F 1150
C                                                                       F 1160
C     COMPUTE ELEMENTS OF STHETA MATRIX                                 F 1170
C                                                                       F 1180
      COFTTA=EXETT/(4.*AM*AM)                                           F 1190
      STHETA(1,1)=COFTTA*A3I*A3I                                        F 1200
      STHETA(1,2)=COFTTA*A3I*A3J                                        F 1210
      STHETA(1,3)=COFTTA*A3I*A3K                                        F 1220
      STHETA(2,1)=COFTTA*A3J*A3I                                        F 1230
      STHETA(2,2)=COFTTA*A3J*A3J                                        F 1240
      STHETA(2,3)=COFTTA*A3J*A3K                                        F 1250
      STHETA(3,1)=COFTTA*A3K*A3I                                        F 1260
      STHETA(3,2)=COFTTA*A3K*A3J                                        F 1270
      STHETA(3,3)=COFTTA*A3K*A3K                                        F 1280
      DO 104 I=1,3                                                      F 1290
         DO 103 J=1,3                                                   F 1300
C                                                                       F 1310
C     COMPUTE ELEMENTS OF FSL MATRIX                                    F 1320
C                                                                       F 1330
            FSL(I,J)=SA(I,J)+SC(I,J)                                    F 1340
C                                                                       F 1350
C     COMPUTE ELEMENTS OF FPLE AND FPLF MATRICES                        F 1360
C                                                                       F 1370
            FPLE(I,J)=SAA(I,J)+SALPHA(I,J)+SBETA(I,J)+SGAMA(I,J)+STHETA(F 1380
     1      I,J)                                                        F 1390
  103    CONTINUE                                                       F 1400
  104 CONTINUE                                                          F 1410
      RETURN                                                            F 1420
C                                                                       F 1430
      END                                                               F 1440
```

SUBROUTINE RHOSEL

```
      SUBROUTINE RHOSEL (M,RHOFL,RHOOEL,RHOO,RHO)                       G  10
C                                                                       G  20
C     THIS SUBROUTINE COMPUTES THE AVERAGE RHO VALUES APPLICABLE TO THE G  30
C     ELEMENT M                                                         G  40
C                                                                       G  50
      COMMON /BLK6/ NP(450,3),P(300),Z(300)                             G  60
      DIMENSION RHOO(300), RHO(300)                                     G  70
      I=NP(M,1)                                                         G  80
      J=NP(M,2)                                                         G  90
      K=NP(M,3)                                                         G 100
      RHOEL=(RHO(I)+RHO(J)+RHO(K))/3.                                   G 110
      RHOOEL=(RHOO(I)+RHOO(J)+RHOO(K))/3.                               G 120
      RETURN                                                            G 130
C                                                                       G 140
      END                                                               G 150
```

SUBROUTINE FSLSK

```
      SUBROUTINE FSLSK (FSL,FPLE,M,DFQ,NPRC,RHO)                        H  10
C                                                                       H  20
C     THIS SUBROUTINE PLACES THE SL,PL AND Q MATRICES FOR DIFFERENT ELEM H  30
C     ENTS INTO THE SK,PKAND QK MATRICES WHICH ARE BANDED AND SYMMETRIC H  40
C                                                                       H  50
      COMMON /BLK3/ SK(300,20)                                          H  60
      COMMON /BLK4/ PK(300,20)                                          H  70
      COMMON /BLK5/ QK(300)                                             H  80
      COMMON /BLK6/ NP(450,3),P(300),Z(300)                             H  90
      DIMENSION FSL(3,3), FPLE(3,3), Q(3), NPRC(300), KP(300), RHO(300) H 100
      II=NP(M,1)                                                        H 110
      LL=NP(M,2)                                                        H 120
      NN=NP(M,3)                                                        H 130
      KP(II)=0                                                          H 140
      KP(LL)=0                                                          H 150
      KP(NN)=0                                                          H 160
      IF (NPRC(II).NE.2.OR.NPRC(LL).NE.2) GO TO 101                     H 170
      KP(II)=1                                                          H 180
      KP(LL)=1                                                          H 190
      IF (Z(II).GT.Z(LL)) DFQ=-DFQ                                      H 200
  101 IF (NPRC(II).NE.2.OR.NPRC(NN).NE.2) GO TO 102                     H 210
      KP(II)=1                                                          H 220
      KP(NN)=1                                                          H 230
      IF (Z(II).GT.Z(NN)) DFQ=-DFQ                                      H 240
  102 IF (NPRC(LL).NE.2.OR.NPRC(NN).NE.2) GO TO 103                     H 250
      KP(LL)=1                                                          H 260
      KP(NN)=1                                                          H 270
      IF (Z(LL).GT.Z(NN)) DFQ=-DFQ                                      H 280
  103 CONTINUE                                                          H 290
      DO 105 J=1,3                                                      H 300
         Q(J)=0.0                                                       H 310
         JJ=NP(M,J)                                                     H 320
         IF (KP(JJ).EQ.1) Q(J)=DFQ*RHO(JJ)                              H 330
         DO 104 K=1,3                                                   H 340
            KK=NP(M,K)                                                  H 350
            IF (KK.LT.JJ) GO TO 104                                     H 360
            KK=KK-JJ+1                                                  H 370
            SK(JJ,KK)=SK(JJ,KK)+FSL(J,K)                                H 380
            PK(JJ,KK)=PK(JJ,KK)+FPLE(J,K)                               H 390
  104    CONTINUE                                                       H 400
  105 QK(JJ)=QK(JJ)+Q(J)                                                H 410
      RETURN                                                            H 420
C                                                                       H 430
      END                                                               H 440
```

SUBROUTINE FSKPSI

```
      SUBROUTINE FSKPSI (PSI,NR,NC,F)                                   I  10
C                                                                       I  20
C     THIS SUBROUTINE MULTIPLIES THE BANDED SYMMETRIC MATRIX SK WITH    I  30
C     MATRIX PSI AND STORES THE RESULT AS MATRIX F                      I  40
C                                                                       I  50
      COMMON /BLK3/ SK(300,20)                                          I  60
      DIMENSION PSI(300), F(300)                                        I  70
      DO 102 I=1,NR                                                     I  80
         F(I)=PSI(I)*SK(I,1)                                            I  90
      DO 102 K=2,NC                                                     I 100
         L=I-K+1                                                        I 110
         IF (L.LT.1) GO TO 101                                          I 120
         F(I)=F(I)+PSI(L)*SK(L,K)                                       I 130
  101    N=I+K-1                                                        I 140
         IF (N.GT.NR) GO TO 102                                         I 150
         F(I)=F(I)+PSI(N)*SK(I,K)                                       I 160
  102 CONTINUE                                                          I 170
      RETURN                                                            I 180
C                                                                       I 190
      END                                                               I 200
```

SUBROUTINE GAUSS

```
      SUBROUTINE GAUSS (NR,NC,F)                                        J  10
C                                                                       J  20
C     THIS SUBROUTINE SOLVES A BANDED SYMMETRIC MATRIX BY GAUSS ELIMINA. J  30
C                                                                       J  40
      COMMON /BLK4/ PK(300,20)                                          J  50
      DIMENSION F(300), AF(300)                                         J  60
      NPM1=NR-1                                                         J  70
      DO 103 I=1,NPM1                                                   J  80
         D=1./PK(I,1)                                                   J  90
         JEND=NR-I+1                                                    J 100
         IF (JEND.GT.NC) JEND=NC                                        J 110
         DO 102 J=2,JEND                                                J 120
            NPN=I+J-1                                                   J 130
            FAC=PK(I,J)*D                                               J 140
            M=0                                                         J 150
            DO 101 K=J,JEND                                             J 160
               M=M+1                                                    J 170
               PK(NPN,M)=PK(NPN,M)-PK(I,K)*FAC                          J 180
  101       CONTINUE                                                    J 190
            F(NPN)=F(NPN)-F(I)*FAC                                      J 200
            PK(I,J)=FAC                                                 J 210
  102    CONTINUE                                                       J 220
         F(I)=F(I)*D                                                    J 230
  103 CONTINUE                                                          J 240
      F(NR)=F(NR)/PK(NR,1)                                              J 250
C                                                                       J 260
```

```
C     BACK SUBSTITUTION                                                 J  270
C                                                                       J  280
      AF(NR)=F(NR)                                                      J  290
      DO 105 I=1,NPM1                                                   J  300
         NPN=NR-I                                                       J  310
         JEND=NR-NPN+1                                                  J  320
         IF (JEND.GT.NC) JEND=NC                                        J  330
         RHS=F(NPN)                                                     J  340
         DO 104 J=2,JEND                                                J  350
            M=NPN+J-1                                                   J  360
            RHS=RHS-PK(NPN,J)*AF(M)                                     J  370
  104    CONTINUE                                                       J  380
  105 AF(NPN)=RHS                                                       J  390
      DO 106 I=1,NR                                                     J  400
  106 F(I)=AF(I)                                                        J  410
      RETURN                                                            J  420
C                                                                       J  430
      END                                                               J  440
```

SUBROUTINE ELVEL

```
      SUBROUTINE ELVEL (M,RLOC,ZLOC,H,AMU,AM)                           K   10
      COMMON /BLK6/ NP(450,3),P(300),Z(300)                             K   20
      COMMON /BLK8/ VR(450),VZ(450),FK(450),RHO(300),C(300)             K   30
      DIMENSION RLOC(3), ZLOC(3), H(300)                                K   40
      I=NP(M,1)                                                         K   50
      J=NP(M,2)                                                         K   60
      K=NP(M,3)                                                         K   70
      XII=RLOC(1)                                                       K   80
      XIJ=RLOC(2)                                                       K   90
      XIK=RLOC(3)                                                       K  100
      TAI=ZLOC(1)                                                       K  110
      TAJ=ZLOC(2)                                                       K  120
      TAK=ZLOC(3)                                                       K  130
      A1I=XIJ*TAK-TAJ*XIK                                               K  140
      A2I=TAJ-TAK                                                       K  150
      A3I=XIK-XIJ                                                       K  160
      A1J=XIK*TAI-TAK*XII                                               K  170
      A2J=TAK-TAI                                                       K  180
      A3J=XII-XIK                                                       K  190
      A1K=XII*TAJ-TAI*XIJ                                               K  200
      A2K=TAI-TAJ                                                       K  210
      A3K=XIJ-XII                                                       K  220
      VR(M)=-(FK(M)/AMU)*((A2I*H(I))+(A2J*H(J))+(A2K*H(K)))/(2.*AM)     K  230
      VZ(M)=-(FK(M)/AMU)*((A3I*H(I))+(A3J*H(J))+(A3K*H(K)))/(2.*AM)     K  240
      RETURN                                                            K  250
C                                                                       K  260
      END                                                               K  270
```

SUBROUTINE SLPL

```
      SUBROUTINE SLPL (RLOC,ZLOC,RBAR,AM,PL,SL,ALPHA,A1,DD,T,A11,EXXFT,E  L   10
     1XXX,EXFTT,RHOEL,XISQ,TASQ,XITA,M)                                   L   20
      COMMON /BLK8/ VR(450),VZ(450),FK(450),RHO(300),C(300)               L   30
C                                                                         L   40
C     THIS SUBROUTINE COMPUTES THE SL AND PL MATRICES                     L   50
C                                                                         L   60
      DIMENSION RLOC(3), ZLOC(3), PL(3,3), SL(3,3), SA(3,3), SB(3,3), SC  L   70
     1(3,3), SF(3,3), SG(3,3), SH(3,3), SI(3,3), SAA(3,3), SALPHA(3,3),   L   80
     2PSRETA(3,3), SGAMA(3,3), STHETA(3,3)                                L   90
      XII=RLOC(1)                                                         L  100
      XIJ=RLOC(2)                                                         L  110
      XIK=RLOC(3)                                                         L  120
      TAI=ZLOC(1)                                                         L  130
      TAJ=ZLOC(2)                                                         L  140
      TAK=ZLOC(3)                                                         L  150
      A1I=XIJ*TAK-TAJ*XIK                                                 L  160
      A2I=TAJ-TAK                                                         L  170
      A3I=XIK-XIJ                                                         L  180
      A1J=XIK*TAI-TAK*XII                                                 L  190
      A2J=TAK-TAI                                                         L  200
      A3J=XII-XIK                                                         L  210
      A1K=XII*TAJ-TAI*XIJ                                                 L  220
      A2K=TAI-TAJ                                                         L  230
      A3K=XIJ-XII                                                         L  240
      AAM=ABS(AM)                                                         L  250
      VV=SQRT(VR(M)*VR(M)+VZ(M)*VZ(M))                                    L  260
      DRR=A1*VV                                                           L  270
      DRZ=0.0                                                             L  280
      DZZ=0.0                                                             L  290
C                                                                         L  300
C     COMPUTE ELEMENTS OF SA MATRIX                                       L  310
C                                                                         L  320
      COFSA=(RBAR*AAM*DRR)/(4.0*AM*AM)                                    L  330
      SA(1,1)=COFSA*A2I*A2I                                               L  340
      SA(1,2)=COFSA*A2I*A2J                                               L  350
      SA(1,3)=COFSA*A2I*A2K                                               L  360
      SA(2,1)=COFSA*A2J*A2I                                               L  370
      SA(2,2)=COFSA*A2J*A2J                                               L  380
      SA(2,3)=COFSA*A2J*A2K                                               L  390
      SA(3,1)=COFSA*A2K*A2I                                               L  400
      SA(3,2)=COFSA*A2K*A2J                                               L  410
      SA(3,3)=COFSA*A2K*A2K                                               L  420
C                                                                         L  430
C     COMPUTE ELEMENTS OF SB MATRIX                                       L  440
C                                                                         L  450
      COFSB=(RBAR*AAM*DRZ)/(4.0*AM*AM)                                    L  460
      SB(1,1)=COFSB*((A3I*A2I)+(A2I*A3I))                                 L  470
      SB(1,2)=COFSB*((A3I*A2J)+(A2I*A3J))                                 L  480
      SB(1,3)=COFSB*((A3I*A2K)+(A2I*A3K))                                 L  490
      SB(2,1)=COFSB*((A3J*A2I)+(A2J*A3I))                                 L  500
      SB(2,2)=COFSB*((A3J*A2J)+(A2J*A3J))                                 L  510
      SB(2,3)=COFSB*((A3J*A2K)+(A2J*A3K))                                 L  520
      SB(3,1)=COFSB*((A3K*A2I)+(A2K*A3I))                                 L  530
      SB(3,2)=COFSB*((A3K*A2J)+(A2K*A3J))                                 L  540
      SB(3,3)=COFSB*((A3K*A2K)+(A2K*A3K))                                 L  550
C                                                                         L  560
C     COMPUTE ELEMENTS OF SC MATRIX                                       L  570
C                                                                         L  580
      COFSC=(RBAR*AAM*DZZ)/(4.0*AM*AM)                                    L  590
      SC(1,1)=COFSC*A3I*A3I                                               L  600
      SC(1,2)=COFSC*A3I*A3J                                               L  610
      SC(1,3)=COFSC*A3I*A3K                                               L  620
      SC(2,1)=COFSC*A3J*A3I                                               L  630
      SC(2,2)=COFSC*A3J*A3J                                               L  640
      SC(2,3)=COFSC*A3J*A3K                                               L  650
      SC(3,1)=COFSC*A3K*A3I                                               L  660
      SC(3,2)=COFSC*A3K*A3J                                               L  670
      SC(3,3)=COFSC*A3K*A3K                                               L  680
C                                                                         L  690
C     COMPUTE ELEMENTS OF SF MATRIX                                       L  700
C                                                                         L  710
      COFSF=VR(M)/(4.0*AM*AM)                                             L  720
      SF(1,1)=COFSF*(A2I*A2I*XISQ+A2I*A3I*XITA)                           L  730
      SF(1,2)=COFSF*(A2J*A2I*XISQ+A2J*A3I*XITA)                           L  740
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      SF(1,3)=COFSF*(A2K*A2I*XISQ+A2K*A3I*XITA)                          L  750
      SF(2,1)=COFSF*(A2I*A2J*XISQ+A2I*A3J*XITA)                          L  760
      SF(2,2)=COFSF*(A2J*A2J*XISQ+A2J*A3J*XITA)                          L  770
      SF(2,3)=COFSF*(A2K*A2J*XISQ+A2K*A3J*XITA)                          L  780
      SF(3,1)=COFSF*(A2I*A2K*XISQ+A2I*A3K*XITA)                          L  790
      SF(3,2)=COFSF*(A2J*A2K*XISQ+A2J*A3K*XITA)                          L  800
      SF(3,3)=COFSF*(A2K*A2K*XISQ+A2K*A3K*XITA)                          L  810
C                                                                        L  820
CC    COMPUTE ELEMENTS OF SG MATRIX                                      L  830
C                                                                        L  840
      COFSG=VZ(M)/(4.0*AM*AM)                                            L  850
      SG(1,1)=COFSG*(A3I*A2I*XISQ+A3I*A3I*XITA)                          L  860
      SG(1,2)=COFSG*(A3J*A2I*XISQ+A3J*A3I*XITA)                          L  870
      SG(1,3)=COFSG*(A3K*A2I*XISQ+A3K*A3I*XITA)                          L  880
      SG(2,1)=COFSG*(A3I*A2J*XISQ+A3I*A3J*XITA)                          L  890
      SG(2,2)=COFSG*(A3J*A2J*XISQ+A3J*A3J*XITA)                          L  900
      SG(2,3)=COFSG*(A3K*A2J*XISQ+A3K*A3J*XITA)                          L  910
      SG(3,1)=COFSG*(A3I*A2K*XISQ+A3I*A3K*XITA)                          L  920
      SG(3,2)=COFSG*(A3J*A2K*XISQ+A3J*A3K*XITA)                          L  930
      SG(3,3)=COFSG*(A3K*A2K*XISQ+A3K*A3K*XITA)                          L  940
C                                                                        L  950
CC    COMPUTE ELEMENTS OF SH MATRIX                                      L  960
C                                                                        L  970
      COFSH=(VR(M)*RBAR*AAM)/(4.0*AM*AM)                                 L  980
      SH(1,1)=A1I*A2I*COFSH                                              L  990
      SH(1,2)=A1I*A2J*COFSH                                              L 1000
      SH(1,3)=A1I*A2K*COFSH                                              L 1010
      SH(2,1)=A1J*A2I*COFSH                                              L 1020
      SH(2,2)=A1J*A2J*COFSH                                              L 1030
      SH(2,3)=A1J*A2K*COFSH                                              L 1040
      SH(3,1)=A1K*A2I*COFSH                                              L 1050
      SH(3,2)=A1K*A2J*COFSH                                              L 1060
      SH(3,3)=A1K*A2K*COFSH                                              L 1070
C                                                                        L 1080
CC    COMPUTE ELEMENTS OF SI MATRIX                                      L 1090
C                                                                        L 1100
      COFSI=(VZ(M)*RRAR*AAM)/(4.0*AM*AM)                                 L 1110
      SI(1,1)=A1I*A3I*COFSI                                              L 1120
      SI(1,2)=A1I*A3J*COFSI                                              L 1130
      SI(1,3)=A1I*A3K*COFSI                                              L 1140
      SI(2,1)=A1J*A3I*COFSI                                              L 1150
      SI(2,2)=A1J*A3J*COFSI                                              L 1160
      SI(2,3)=A1J*A3K*COFSI                                              L 1170
      SI(3,1)=A1K*A3I*COFSI                                              L 1180
      SI(3,2)=A1K*A3J*COFSI                                              L 1190
      SI(3,3)=A1K*A3K*COFSI                                              L 1200
C                                                                        L 1210
CC    COMPUTE ELEMENTS OF SAA MATRIX                                     L 1220
C                                                                        L 1230
      COFSAA=RRAR/(4.0*AM*AM)                                            L 1240
       SAA(1,1)=(AAM*A1I*A1I+A2I*A2I*XISQ+(A2I*A3I+A3I*A2I)*XITA+A3I*A3I* L 1250
     1TASQ)*COFSAA                                                       L 1260
       SAA(1,2)=(AAM*A1J*A1I+A2J*A2I*XISQ+(A2J*A3I+A3J*A2I)*XITA+A3J*A3I* L 1270
     1TASQ)*COFSAA                                                       L 1280
       SAA(1,3)=(AAM*A1K*A1I+A2K*A2I*XISQ+(A2K*A3I+A3K*A2I)*XITA+A3K*A3I* L 1290
     1TASQ)*COFSAA                                                       L 1300
       SAA(2,1)=(AAM*A1I*A1J+A2I*A2J*XISQ+(A2I*A3J+A3I*A2J)*XITA+A3I*A3J* L 1310
     1TASQ)*COFSAA                                                       L 1320
       SAA(2,2)=(AAM*A1J*A1J+A2J*A2J*XISQ+(A2J*A3J+A3J*A2J)*XITA+A3J*A3J* L 1330
     1TASQ)*COFSAA                                                       L 1340
       SAA(2,3)=(AAM*A1K*A1J+A2K*A2J*XISQ+(A2K*A3J+A3K*A2J)*XITA+A3K*A3J* L 1350
     1TASQ)*COFSAA                                                       L 1360
       SAA(3,1)=(AAM*A1I*A1K+A2I*A2K*XISQ+(A2I*A3K+A3I*A2K)*XITA+A3I*A3K* L 1370
     1TASQ)*COFSAA                                                       L 1380
       SAA(3,2)=(AAM*A1J*A1K+A2J*A2K*XISQ+(A2J*A3K+A3J*A2K)*XITA+A3J*A3K* L 1390
     1TASQ)*COFSAA                                                       L 1400
       SAA(3,3)=(AAM*A1K*A1K+A2K*A2K*XISQ+(A2K*A3K+A3K*A2K)*XITA+A3K*A3K* L 1410
     1TASQ)*COFSAA                                                       L 1420
C                                                                        L 1430
CC    COMPUTE ELEMENTS OF SALPHA MATRIX                                  L 1440
C                                                                        L 1450
      SALPHA(1,1)=(A2I*A1I+A1I*A2I)*XISQ+(A3I*A1I+A1I*A3I)*XITA          L 1460
      SALPHA(1,2)=(A2I*A1J+A1I*A2J)*XISQ+(A3I*A1J+A1I*A3J)*XITA          L 1470
      SALPHA(1,3)=(A2I*A1K+A1I*A2K)*XISQ+(A3I*A1K+A1I*A3K)*XITA          L 1480
      SALPHA(2,1)=(A2J*A1I+A1J*A2I)*XISQ+(A3J*A1I+A1J*A3I)*XITA          L 1490
      SALPHA(2,2)=(A2J*A1J+A1J*A2J)*XISQ+(A3J*A1J+A1J*A3J)*XITA          L 1500
      SALPHA(2,3)=(A2J*A1K+A1J*A2K)*XISQ+(A3J*A1K+A1J*A3K)*XITA          L 1510
      SALPHA(3,1)=(A2K*A1I+A1K*A2I)*XISQ+(A3K*A1I+A1K*A3I)*XITA          L 1520
      SALPHA(3,2)=(A2K*A1J+A1K*A2J)*XISQ+(A3K*A1J+A1K*A3J)*XITA          L 1530
      SALPHA(3,3)=(A2K*A1K+A1K*A2K)*XISQ+(A3K*A1K+A1K*A3K)*XITA          L 1540
      DO 102 I=1,3                                                       L 1550
         DO 101 J=1,3                                                    L 1560
            SALPHA(I,J)=SALPHA(I,J)/(4.0*AM*AM)                          L 1570
  101    CONTINUE                                                        L 1580
  102 CONTINUE                                                           L 1590
C                                                                        L 1600
CC    COMPUTE ELEMENTS OF SBETA MATRIX                                   L 1610
C                                                                        L 1620
      COFBTA=EXXET/(4.*AM*AM)                                            L 1630
      SBETA(1,1)=COFBTA*(A2I*A3I+A3I*A2I)                                L 1640
      SBETA(1,2)=COFBTA*(A2I*A3J+A3I*A2J)                                L 1650
      SBETA(1,3)=COFBTA*(A2I*A3K+A3I*A2K)                                L 1660
      SBETA(2,1)=COFBTA*(A2J*A3I+A3J*A2I)                                L 1670
      SBETA(2,2)=COFBTA*(A2J*A3J+A3J*A2J)                                L 1680
      SBETA(2,3)=COFBTA*(A2J*A3K+A3J*A2K)                                L 1690
      SBETA(3,1)=COFBTA*(A2K*A3I+A3K*A2I)                                L 1700
      SBETA(3,2)=COFBTA*(A2K*A3J+A3K*A2J)                                L 1710
      SBETA(3,3)=COFBTA*(A2K*A3K+A3K*A2K)                                L 1720
C                                                                        L 1730
CC    COMPUTE ELEMENTS OF SGAMA MATRIX                                   L 1740
C                                                                        L 1750
      COFGMA=FXXX/(4.*AM*AM)                                             L 1760
      SGAMA(1,1)=COFGMA*A2I*A2I                                          L 1770
      SGAMA(1,2)=COFGMA*A2I*A2J                                          L 1780
      SGAMA(1,3)=COFGMA*A2I*A2K                                          L 1790
      SGAMA(2,1)=COFGMA*A2J*A2I                                          L 1800
      SGAMA(2,2)=COFGMA*A2J*A2J                                          L 1810
      SGAMA(2,3)=COFGMA*A2J*A2K                                          L 1820
      SGAMA(3,1)=COFGMA*A2K*A2I                                          L 1830
      SGAMA(3,2)=COFGMA*A2K*A2J                                          L 1840
      SGAMA(3,3)=COFGMA*A2K*A2K                                          L 1850
C                                                                        L 1860
CC    COMPUTE ELEMENTS OF STHETA MATRIX                                  L 1870
C                                                                        L 1880
      COFTTA=EXETT/(4.*AM*AM)                                            L 1890
      STHETA(1,1)=COFTTA*A3I*A3I                                         L 1900
      STHETA(1,2)=COFTTA*A3I*A3J                                         L 1910
      STHETA(1,3)=COFTTA*A3I*A3K                                         L 1920
      STHETA(2,1)=COFTTA*A3J*A3I                                         L 1930
      STHETA(2,2)=COFTTA*A3J*A3J                                         L 1940
      STHETA(2,3)=COFTTA*A3J*A3K                                         L 1950
      STHETA(3,1)=COFTTA*A3K*A3I                                         L 1960
      STHETA(3,2)=COFTTA*A3K*A3J                                         L 1970
      STHETA(3,3)=COFTTA*A3K*A3K                                         L 1980
C                                                                        L 1990
CC    COMBINE THESE MATRICES TO GET SL AND PL MATRICES                   L 2000
C                                                                        L 2010
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```
      DO 104 I=1,3                                                      L 2020
         DO 103 J=1,3                                                   L 2030
            PL(I,J)=SBA(I,J)+SALPHA(I,J)+SRETA(I,J)+SGAMA(I,J)+STHETA(I, L 2040
     1      J)                                                          L 2050
            SL(I,J)=SA(I,J)+SR(I,J)+SC(I,J)+SF(I,J)+SG(I,J)+SM(I,J)+SI(I L 2060
     1      ,J)                                                         L 2070
  103    CONTINUE                                                       L 2080
  104 CONTINUE                                                         L 2090
      RETURN                                                           L 2100
C                                                                      L 2110
      END                                                              L 2120
```

SUBROUTINE SLSK

```
      SUBROUTINE SLSK (SL,PL,DFQ,M,NPBC,PSI,IBAND)                     M   10
C                                                                      M   20
C     THIS SUBROUTINE PLACES THE SL,PL AND Q MATRICES FOR DIFFERENT ELEM M   30
C     ENTS INTO THE SK,PKAND QK MATRICES WHICH ARE BANDED AND SYMMETRIC  M   40
C                                                                      M   50
      COMMON /BLK3/ SK(300,20)                                         M   60
      COMMON /BLK4/ PK(300,20)                                         M   70
      COMMON /BLK5/ QK(300)                                            M   80
      COMMON /BLK6/ NP(450,3),R(300),Z(300)                            M   90
      COMMON /BLK7/ PHIO(300)                                          M  100
      DIMENSION SL(3,3), PL(3,3), Q(3), NPBC(300), KP(300), PSIH(300), P M  110
     1SI(300)                                                          M  120
      II=NP(M,1)                                                       M  130
      LL=NP(M,2)                                                       M  140
      NN=NP(M,3)                                                       M  150
      KP(II)=0                                                         M  160
      KP(LL)=0                                                         M  170
      KP(NN)=0                                                         M  180
      IF (NPBC(II).NE.2.OR.NPBC(LL).NE.2) GO TO 101                    M  190
      KP(II)=1                                                         M  200
      KP(LL)=1                                                         M  210
      IF (Z(II).GT.Z(LL)) DFQ=-DFQ                                     M  220
      PSIB(II)=(PSI(II)/3.0)+(PSI(LL)/6.0)                             M  230
      PSIB(LL)=(PSI(II)/6.0)+(PSI(LL)/3.0)                             M  240
  101 IF (NPBC(II).NE.2.OR.NPBC(NN).NE.2) GO TO 102                    M  250
      KP(II)=1                                                         M  260
      KP(NN)=1                                                         M  270
      IF (Z(II).GT.Z(NN)) DFQ=-DFQ                                     M  280
      PSIB(II)=(PSI(II)/3.0)+(PSI(NN)/6.0)                             M  290
      PSIB(NN)=(PSI(II)/6.0)+(PSI(NN)/3.0)                             M  300
  102 IF (NPBC(LL).NE.2.OR.NPBC(NN).NE.2) GO TO 103                    M  310
      KP(LL)=1                                                         M  320
      KP(NN)=1                                                         M  330
      IF (Z(LL).GT.Z(NN)) DFQ=-DFQ                                     M  340
      PSIB(LL)=(PSI(LL)/3.0)+(PSI(NN)/6.0)                             M  350
      PSIB(NN)=(PSI(LL)/6.0)+(PSI(NN)/3.0)                             M  360
  103 CONTINUE                                                         M  370
      DO 105 J=1,3                                                     M  380
         Q(J)=0.0                                                      M  390
         JJ=NP(M,J)                                                    M  400
         IF (KP(JJ).EQ.1) Q(J)=DFQ*PSIB(JJ)*((1./PHIO(JJ))-1.)*2.      M  410
         DO 104 K=1,3                                                  M  420
            KK=NP(M,K)                                                 M  430
            KK=KK-JJ+((IBAND+1)/2)                                     M  440
            SK(JJ,KK)=SK(JJ,KK)+SL(J,K)                                M  450
            PK(JJ,KK)=PK(JJ,KK)+PL(J,K)                                M  460
  104    CONTINUE                                                      M  470
  105 QK(JJ)=QK(JJ)+Q(J)                                               M  480
      RETURN                                                           M  490
C                                                                      M  500
      END                                                              M  510
```

SUBROUTINE BSOLVE

```
      SUBROUTINE BSOLVE (N,M,V)                                        N   10
      COMMON /BLK4/ PK(300,20)                                         N   20
      DIMENSION V(300)                                                 N   30
C                                                                      N   40
C     BSOLVE WORKS FOR FOR  UNSYMMETRIC BANDED MATRICES.               N   50
C     BSOLVE IS EFFECTIVE IN SOLVING THE MATRIX EQUATION AX = R WHEN THE N   60
C     MATRIX A IS LARGE AND SPARSE SUCH THAT A NARROWUNSYMMETRIC BAND  N   70
C     CENTERED ON THE MAIN DIAGONAL INCLUDES ALL THE NON-ZERO ELEMENTS. N   80
C     ARGUMENT N IS THE ORDER OF A, AND M IS THE WIDTH OF THE BAND.    N   90
C     NECESSARILY AN ODD NUMBER OF ELEMENTS. BSOLVE IS VERY EFFICIENT  N  100
C     BECAUSE IT OPERATES ONLY ON THE BAND PORTION OF MATRIX A, GIVEN   N  110
C     IN THE N BY M ARRAY PK. THE BAND ELEMENTS OF A GIVEN ROW OF A    N  120
C     APPEAR IN THE SAME ROW OF PK BUT SHIFTED SUCH THAT ELEMENT A(I,J) N  130
C     BECOMES PK(I,J-I+(M+1)/2). ALL BAND ELEMENTS WHETHER ZERO OR NON- N  140
C     ZERO MUST BE GIVEN.THE VALUES OF UNDEFINED ELEMENTS OF PK,SUCH   N  150
C     AS PK(1,1) AND PK(N,M) ETC. ARE IRRLEVANT. THE ARRAY V INITIALLY N  160
C     CONTAINS THE VECTOR B. AFTER SOLUTION, THE ARRAY V CONTAINS THE  N  170
C     ANSWER VECTOR X.THE CONTENTS OF PK ARE DESTROYED DURING SOLUTION N  180
C     WHICH IS DONE BY GAUSS ELIMINATION WITH ROW INTERCHANGES, FOLLOWED N  190
C     BY BACK SUBSTITUTION.                                            N  200
C                                                                      N  210
C     THE ROW DIMENSION OF PK AS WELL AS THE DIMENSION OF V MUST BE NO  N  220
C     LESS THAN N. THE COLUMN DIMENSION OF PK MUST BE NO LESS THAN M.  N  230
C     SHIFT TOP (M-1)/2 ROWS AND PLACE NEEDED ZEROES                   N  240
C                                                                      N  250
      LR=(M-1)/2                                                       N  260
      DO 102 L=1,LR                                                    N  270
         IM=LR-L+1                                                     N  280
      DO 102 I=1,IM                                                    N  290
         DO 101 J=2,M                                                  N  300
  101    PK(L,J-1)=PK(L,J)                                             N  310
         KN=N-L                                                        N  320
         KM=M-I                                                        N  330
         PK(L,M)=0.0                                                   N  340
  102 PK(KN+1,KM+1)=0.0                                                N  350
C                                                                      N  360
C     GAUSS ELIMINATION WITH ROW INTERCHANGES                          N  370
C                                                                      N  380
      LR=LR+1                                                          N  390
      IM=N-1                                                           N  400
      DO 112 I=1,IM                                                    N  410
         NPIV=I                                                        N  420
         LS=I+1                                                        N  430
         DO 104 L=LS,LR                                                N  440
            IF (ABS(PK(L,1))-ABS(PK(NPIV,1))) 104,104,103              N  450
  103       NPIV=L                                                     N  460
  104    CONTINUE                                                      N  470
         IF (NPIV-I) 107,107,105                                       N  480
  105    DO 106 J=1,M                                                  N  490
            TEMP=PK(I,J)                                               N  500
            PK(I,J)=PK(NPIV,J)                                         N  510
  106    PK(NPIV,J)=TEMP                                               N  520
         TEMP=V(I)                                                     N  530
         V(I)=V(NPIV)                                                  N  540
```

```
      V(NPIV)=TEMP                                                    N  550
  107 V(I)=V(I)/PK(I,1)                                               N  560
      DO 108 J=2,M                                                    N  570
  108 PK(I,J)=PK(I,J)/PK(I,1)                                         N  580
      DO 110 L=LS,LR                                                  N  590
         TEMP=PK(L,1)                                                 N  600
         V(L)=V(L)-TEMP*V(I)                                          N  610
         DO 109 J=2,M                                                 N  620
  109    PK(L,J-1)=PK(L,J)-TEMP*PK(I,J)                               N  630
  110 PK(L,M)=0.0                                                     N  640
      IF (LR-N) 111,112,112                                           N  650
  111 LR=LR+1                                                         N  660
  112 CONTINUE                                                        N  670
      V(N)=V(N)/PK(N,1)                                               N  680
C                                                                     N  690
C     BACK SUBSTITUTION                                               N  700
C                                                                     N  710
      JM=2                                                            N  720
      DO 115 I=1,IM                                                   N  730
         L=N-I                                                        N  740
         DO 113 J=2,JM                                                N  750
            KM=L+J                                                    N  760
  113    V(L)=V(L)-PK(L,J)*V(KM-1)                                    N  770
         IF (JM-M) 114,115,115                                        N  780
  114    JM=JM+1                                                      N  790
  115 CONTINUE                                                        N  800
      RETURN                                                          N  810
C                                                                     N  820
      END                                                             N  830
```

SUBROUTINE SKPSI

```
      SUBROUTINE SKPSI (PSI,NR,NC,F)                                  0   10
C                                                                     0   20
C     THIS SURROUTINE MULTIPLIES THE BANDED SYMMETRIC MATRIX SK WITH  0   30
C     MATRIX PSI AND STORES THE RESULT AS MATRIX F                    0   40
C                                                                     0   50
      COMMON /BLK3/ SK(300,20)                                        0   60
      DIMENSION PSI(300), F(300)                                      0   70
      M=(NC+1)/2                                                      0   80
      DO 102 I=1,NR                                                   0   90
         F(I)=PSI(I)*SK(I,M)                                          0  100
C                                                                     0  110
      DO 102 K=2,M                                                    0  120
         L=I-K+1                                                      0  130
         IF (L.LT.1) GO TO 101                                        0  140
         LL=M-K+1                                                     0  150
         F(I)=F(I)+PSI(L)*SK(I,LL)                                    0  160
  101    N=I+K-1                                                      0  170
         IF(N.GT.NR) GO TO 102                                        0  180
         NN=K+M-1                                                     0  190
         F(I)=F(I)+PSI(N)*SK(I,NN)                                    0  200
  102 CONTINUE                                                        0  210
      RETURN                                                          0  220
C                                                                     0  230
      END                                                             0  240
```

PROGRAM MESH

```
      PROGRAM MESH7 (INPUT,OUTPUT,PUNCH,F(LMPL,TAPE5=INPUT,TAPE6=OUTPUT,     A   10
     1TAPE8=PUNCH,DEBUG=OUTPUT)                                              A   20
C                                                                            A   30
C     $    DEBUG                                                           A   40
C     $    ARRAYS                                                          A   50
C                                                                            A   60
      COMMON /BLK1/ JMEM(300),MEMJT(2000),JNT(300)                           A   70
      DIMENSION JT(2000)                                                     A   80
C                                                                            A   90
C     READ AND INITIALIZATION OF DATA                                        A  100
C                                                                            A  110
      READ (5,139) NCON                                                      A  120
      WRITE (6,161)                                                          A  130
      WRITE (6,139) NCON                                                     A  140
      READ (5,139) NUMLPS                                                    A  150
      WRITE (6,140)                                                          A  160
      WRITE (6,139) NUMLPS                                                   A  170
C                                                                            A  180
      WRITE (6,142)                                                          A  190
      READ (5,141) XMIN,XMAX,YMIN,YMAX                                       A  200
      WRITE (6,141) XMIN,XMAX,YMIN,YMAX                                      A  210
C                                                                            A  220
      WRITE (6,156)                                                          A  230
      READ (5,157) IPUNCH                                                    A  240
      WRITE (6,157) IPUNCH                                                   A  250
C                                                                            A  260
      DO 101 I=1,NUMLPS                                                      A  270
         WRITE (6,143) I                                                     A  280
         WRITE (6,145)                                                       A  290
         READ (5,144) NDIV(I,1),NDIV(I,2)                                    A  300
         WRITE (6,144) NDIV(I,1),NDIV(I,2)                                   A  310
C                                                                            A  320
         WRITE (6,146)                                                       A  330
         READ (5,147) ((JOIN(I,J,K),K=1,2),J=1,4)                            A  340
         WRITE (6,147) ((JOIN(I,J,K),K=1,2),J=1,4)                           A  350
C                                                                            A  360
         WRITE (6,148)                                                       A  370
         READ (5,149) (XCOR(I,J),YCOR(I,J),J=1,8)                            A  380
         WRITE (6,149) (XCOR(I,J),YCOR(I,J),J=1,8)                           A  390
C                                                                            A  400
  101 CONTINUE                                                               A  410
C                                                                            A  420
  102 CONTINUE                                                               A  430
C                                                                            A  440
C                                                                            A  450
      DO 103 I=1,NUMLPS                                                      A  460
         NDIV(I,3)=NDIV(I,1)                                                 A  470
         NDIV(I,4)=NDIV(I,2)                                                 A  480
  103 CONTINUE                                                               A  490
      DUM=CHEK(4)                                                            A  500
C                                                                            A  510
C     CALCULATE NUMBER OF NODAL POINTS                                       A  520
C                                                                            A  530
      NUMNP=0                                                                A  540
C                                                                            A  550
      DO 106 I=1,NUMLPS                                                      A  560
         NUMNP=NUMNP+(NDIV(I,1)+1)*(NDIV(I,2)+1)                             A  570
C                                                                            A  580
         J1=4                                                                A  590
C                                                                            A  600
      DO 105 J=1,4                                                           A  610
         IF (JOIN(I,J,1).EQ.0) GO TO 104                                     A  620
         NUMNP=NUMNP-(NDIV(I,J)+1)                                           A  630
         IF (JOIN(I,J1,1).NE.0) NUMNP=NUMNP+1                                A  640
  104    CONTINUE                                                            A  650
         J1=J                                                                A  660
C                                                                            A  670
  105    CONTINUE                                                            A  680
  106 CONTINUE                                                               A  690
C                                                                            A  700
      KT=1                                                                   A  710
  107 CONTINUE                                                               A  720
C                                                                            A  730
      INP=0                                                                  A  740
C                                                                            A  750
      IEL=0                                                                  A  760
C                                                                            A  770
      DO 125 I=1,NUMLPS                                                      A  780
C                                                                            A  790
         I1=NDIV(I,1)                                                        A  800
         I2=I1+1                                                             A  810
C                                                                            A  820
         I4=NDIV(I,2)                                                        A  830
         I5=I4+1                                                             A  840
C                                                                            A  850
         I7=I2*I5                                                            A  860
         IA=I1*I4                                                            A  870
C                                                                            A  880
C     CALCULATE SIDE ARRAYS                                                  A  890
C                                                                            A  900
         JRGN=1                                                              A  910
         JEND=I2                                                             A  920
C                                                                            A  930
         J2=I7-I2                                                            A  940
         J4=I2+1                                                             A  950
C                                                                            A  960
         DO 108 J=JRGN,JEND                                                  A  970
            J4=J4-1                                                          A  980
            LNR(I,1,J)=J                                                     A  990
            LNR(I,3,J4)=J2+J                                                 A 1000
  108    CONTINUE                                                            A 1010
C                                                                            A 1020
C                                                                            A 1030
         JRGN=1                                                              A 1040
         JEND=I5                                                             A 1050
C                                                                            A 1060
         J4=I5+1                                                             A 1070
C                                                                            A 1080
         DO 109 J=JRGN,JEND                                                  A 1090
            J4=J4-1                                                          A 1100
            LNR(I,2,J)=J*I2                                                  A 1110
            LNR(I,4,J4)=(J-1)*I2+1                                           A 1120
  109    CONTINUE                                                            A 1130
C                                                                            A 1140
C                                                                            A 1150
C     CALCULATE NPN ARRAY                                                    A 1160
C                                                                            A 1170
         JRGN=1                                                              A 1180
         JEND=I7                                                             A 1190
C                                                                            A 1200
         DO 110 J=JRGN,JEND                                                  A 1210
            NPN(J)=0                                                         A 1220
  110    CONTINUE                                                            A 1230
C                                                                            A 1240
         DO 112 J=1,4                                                        A 1250
            IF (JOIN(I,J,1).EQ.0) GO TO 112                                  A 1260
C                                                                            A 1270
```

```
            J1=JOIN(I,J,1)                                              A 1280
            J2=JOIN(I,J,2)                                              A 1290
C                                                                       A 1300
            KRGN=1                                                      A 1310
            KEND=NDIV(I,J)+1                                            A 1320
            K2=KEND+1                                                   A 1330
C                                                                       A 1340
            DO 111 K=KRGN,KEND                                          A 1350
               K1=LNP(I,J,K)                                            A 1360
               K2=K2-1                                                  A 1370
               NPN(K1)=LNP(J1,J2,K2)                                    A 1380
  111       CONTINUE                                                    A 1390
C                                                                       A 1400
C                                                                       A 1410
  112    CONTINUE                                                       A 1420
C                                                                       A 1430
         JRGN=1                                                         A 1440
         JEND=I7                                                        A 1450
         DO 113 J=JRGN,JEND                                             A 1460
            IF (NPN(J).NE.0) GO TO 113                                  A 1470
            INP=INP+1                                                   A 1480
            NPN(J)=INP                                                  A 1490
  113    CONTINUE                                                       A 1500
C                                                                       A 1510
C                                                                       A 1520
         WRITE (6,159)                                                  A 1530
         WRITE (6,158) (NPN(J),J=1,I7)                                  A 1540
C                                                                       A 1550
C                                                                       A 1560
C     FORM LNP ARRAY                                                    A 1570
C                                                                       A 1580
         JRGN=1                                                         A 1590
         JEND=I2                                                        A 1600
C                                                                       A 1610
         DO 114 J=JRGN,JEND                                             A 1620
            J1=LNP(I,1,J)                                               A 1630
            J3=LNP(I,3,J)                                               A 1640
C                                                                       A 1650
            LNP(I,1,J)=NPN(J1)                                          A 1660
            LNP(I,3,J)=NPN(J3)                                          A 1670
C                                                                       A 1680
  114    CONTINUE                                                       A 1690
C                                                                       A 1700
         JRGN=1                                                         A 1710
         JEND=I5                                                        A 1720
C                                                                       A 1730
         DO 115 J=JRGN,JEND                                             A 1740
            J2=LNP(I,2,J)                                               A 1750
            J4=LNP(I,4,J)                                               A 1760
C                                                                       A 1770
            LNP(I,2,J)=NPN(J2)                                          A 1780
            LNP(I,4,J)=NPN(J4)                                          A 1790
  115    CONTINUE                                                       A 1800
         WRITE (6,159)                                                  A 1810
         WRITE (6,158) (LNP(I,1,J),J=1,I2)                              A 1820
         WRITE (6,158) (LNP(I,2,J),J=1,I5)                              A 1830
         WRITE (6,158) (LNP(I,3,J),J=1,I2)                              A 1840
         WRITE (6,158) (LNP(I,4,J),J=1,I5)                              A 1850
         WRITE (6,159)                                                  A 1860
C                                                                       A 1870
C                                                                       A 1880
C     CALCULATE NODAL POINT COORDINATES                                 A 1890
C                                                                       A 1900
         R=I1                                                           A 1910
         DX=1.0/R                                                       A 1920
         R=I4                                                           A 1930
         DY=1.0/R                                                       A 1940
C                                                                       A 1950
         JRGN=1                                                         A 1960
         JEND=I5                                                        A 1970
C                                                                       A 1980
         KRGN=1                                                         A 1990
         KEND=I2                                                        A 2000
C                                                                       A 2010
         K1=0                                                           A 2020
C                                                                       A 2030
         DO 118 J=JRGN,JEND                                             A 2040
            R=J-1                                                       A 2050
            RY=R*DY                                                     A 2060
C                                                                       A 2070
            DO 117 K=KRGN,KEND                                          A 2080
               R=K-1                                                    A 2090
               RX=R*DX                                                  A 2100
               RN(1)=+1.0*(1.0-RX)*(1.0-RY)*(1.0-2.0*RX-2.0*RY)         A 2110
               RN(2)=+4.0*(RX)*(1.0-RX)*(1.0-RY)                        A 2120
               RN(3)=-1.0*(RX)*(1.0-RY)*(1.0-2.0*RX+2.0*RY)             A 2130
               RN(4)=+4.0*(RX)*(RY)*(1.0-RY)                            A 2140
               RN(5)=-1.0*(RX)*(RY)*(3.0-2.0*RX-2.0*RY)                 A 2150
               RN(6)=+4.0*(RX)*(1.0-RX)*(RY)                            A 2160
               RN(7)=-1.0*(1.0-RX)*(RY)*(1.0+2.0*RX-2.0*RY)             A 2170
               RN(8)=+4.0*(1.0-RX)*(RY)*(1.0-RY)                        A 2180
               K1=K1+1                                                  A 2190
               K2=NPN(K1)                                               A 2200
               XORD(K2)=0.0                                             A 2210
               YORD(K2)=0.0                                             A 2220
               DO 116 L=1,8                                             A 2230
                  XORD(K2)=XORD(K2)+RN(L)*XCOR(I,L)                     A 2240
                  YORD(K2)=YORD(K2)+RN(L)*YCOR(I,L)                     A 2250
  116          CONTINUE                                                 A 2260
C                                                                       A 2270
  117       CONTINUE                                                    A 2280
  118    CONTINUE                                                       A 2290
C                                                                       A 2300
C     CALCULATION OF NP ARRAY                                           A 2310
C                                                                       A 2320
         JRGN=1                                                         A 2330
         JEND=I4                                                        A 2340
         KRGN=1                                                         A 2350
         KEND=I1                                                        A 2360
C                                                                       A 2370
         DO 124 J=JRGN,JEND                                             A 2380
            DO 123 K=KRGN,KEND                                          A 2390
C                                                                       A 2400
               IEL=IEL+2                                                A 2410
               N1=IEL-1                                                 A 2420
               N2=IEL                                                   A 2430
C                                                                       A 2440
               K1=(J-1)*I2+(K-1)+1                                      A 2450
               K2=K1+1                                                  A 2460
               K3=K1+I2                                                 A 2470
               K4=K3+1                                                  A 2480
C                                                                       A 2490
               K1=NPN(K1)                                               A 2500
               K2=NPN(K2)                                               A 2510
               K3=NPN(K3)                                               A 2520
               K4=NPN(K4)                                               A 2530
C                                                                       A 2540
               D1=(XORD(K4)-XORD(K1))**2+(YORD(K4)-YORD(K1))**2         A 2550
               D1=D1+0.000001                                           A 2560
               D2=(XORD(K3)-XORD(K2))**2+(YORD(K3)-YORD(K2))**2         A 2570
C                                                                       A 2580
               IF (KT-1) 119,119,120                                    A 2590
  119          CONTINUE                                                 A 2600
               IF (D2.LT.D1) GO TO 122                                  A 2610
```

```
            GO TO 121                                                   A 2620
  120       CONTINUE                                                    A 2630
            IF (D2.GE.D1) GO TO 122                                     A 2640
  121       CONTINUE                                                    A 2650
C                                                                       A 2660
            NP(N1,1)=K1                                                 A 2670
            NP(N1,2)=K4                                                 A 2680
            NP(N1,3)=K3                                                 A 2690
C                                                                       A 2700
            NP(N2,1)=K1                                                 A 2710
            NP(N2,2)=K2                                                 A 2720
            NP(N2,3)=K4                                                 A 2730
C                                                                       A 2740
            GO TO 123                                                   A 2750
  122       CONTINUE                                                    A 2760
C                                                                       A 2770
            NP(N1,1)=K1                                                 A 2780
            NP(N1,2)=K2                                                 A 2790
            NP(N1,3)=K3                                                 A 2800
C                                                                       A 2810
            NP(N2,1)=K2                                                 A 2820
            NP(N2,2)=K4                                                 A 2830
            NP(N2,3)=K3                                                 A 2840
C                                                                       A 2850
  123       CONTINUE                                                    A 2860
  124    CONTINUE                                                       A 2870
C                                                                       A 2880
C                                                                       A 2890
  125 CONTINUE                                                          A 2900
      NUMEL=IEL                                                         A 2910
C                                                                       A 2920
C     OUTPUT OF DATA                                                    A 2930
C                                                                       A 2940
C                                                                       A 2950
      IF (KT.GT.1) GO TO 130                                            A 2960
      DO 126 I=1,NUMEL                                                  A 2970
         NP(I,4)=0                                                      A 2980
  126 CONTINUE                                                          A 2990
      K=0                                                               A 3000
      DO 128 J=1,4                                                      A 3010
         DO 127 I=1,NUMEL                                               A 3020
            K=K+1                                                       A 3030
            JT(K)=NP(I,J)                                               A 3040
  127    CONTINUE                                                       A 3050
  128 CONTINUE                                                          A 3060
      CALL SETUP (NUMNP,NUMEL,NCON,JT,IDIFF)                            A 3070
      CALL OPTNUM (NUMNP,NUMEL,NCON,IDIFF)                              A 3080
      WRITE (6,154)                                                     A 3090
      WRITE (6,155) NUMNP,NUMEL                                         A 3100
      WRITE (6,163)                                                     A 3110
      WRITE (6,162) (J,JNT(J),J=1,NUMNP)                                A 3120
      WRITE (8,162) (J,JNT(J),J=1,NUMNP)                                A 3130
      WRITE (6,150)                                                     A 3140
      DO 129 I=1,NUMNP                                                  A 3150
         WRITE (6,151) JNT(I),XORD(I),YORD(I)                           A 3160
  129 CONTINUE                                                          A 3170
C                                                                       A 3180
  130 CONTINUE                                                          A 3190
      WRITE (6,152)                                                     A 3200
      DO 131 I=1,NUMEL                                                  A 3210
         WRITE (6,153) I,(JNT(NP(I,J)),J=1,3)                           A 3220
  131 CONTINUE                                                          A 3230
C                                                                       A 3240
C                                                                       A 3250
      IF (IPUNCH.NE.8) GO TO 135                                        A 3260
      IF (KT.GT.1) GO TO 133                                            A 3270
      WRITE (8,155) NUMNP,NUMEL                                         A 3280
      DO 132 I=1,NUMNP                                                  A 3290
         WRITE (8,151) JNT(I),XORD(I),YORD(I)                           A 3300
  132 CONTINUE                                                          A 3310
  133 CONTINUE                                                          A 3320
      DO 134 I=1,NUMEL                                                  A 3330
         WRITE (8,153) I,(JNT(NP(I,J)),J=1,3)                           A 3340
  134 CONTINUE                                                          A 3350
  135 CONTINUE                                                          A 3360
      CALL SET (0.0,1.0,0.0,1.0,XMIN,XMAX,YMIN,YMAX,1)                  A 3370
C                                                                       A 3380
      DO 136 I=1,NUMEL                                                  A 3390
         I1=NP(I,1)                                                     A 3400
         I2=NP(I,2)                                                     A 3410
         I3=NP(I,3)                                                     A 3420
C                                                                       A 3430
         CALL POINT (XORD(I1),YORD(I1))                                 A 3440
         CALL VECTOR (XORD(I2),YORD(I2))                                A 3450
         CALL VECTOR (XORD(I3),YORD(I3))                                A 3460
         CALL VECTOR (XORD(I1),YORD(I1))                                A 3470
  136 CONTINUE                                                          A 3480
C                                                                       A 3490
      CALL FRAME                                                        A 3500
C                                                                       A 3510
      KT=KT+1                                                           A 3520
      IF (KT.LE.2) GO TO 107                                            A 3530
C                                                                       A 3540
      READ (5,160) IEND                                                 A 3550
      IF (IEND.EQ.0) GO TO 138                                          A 3560
C                                                                       A 3570
      WRITE (6,145)                                                     A 3580
      DO 137 I=1,NUMLPS                                                 A 3590
         READ (5,144) NDIV(I,1),NDIV(I,2)                               A 3600
         WRITE (6,144) NDIV(I,1),NDIV(I,2)                              A 3610
  137 CONTINUE                                                          A 3620
C                                                                       A 3630
      GO TO 102                                                         A 3640
C                                                                       A 3650
C                                                                       A 3660
  138 CONTINUE                                                          A 3670
C                                                                       A 3680
      STOP                                                              A 3690
C                                                                       A 3700
C     FORMAT STATEMENTS                                                 A 3710
C                                                                       A 3720
C                                                                       A 3730
  139 FORMAT (I10)                                                      A 3740
  140 FORMAT (10H1   NUMLPS)                                            A 3750
  141 FORMAT (4F10.3)                                                   A 3760
  142 FORMAT (40H0      XMIN       XMAX       YMIN       YMAX)         A 3770
  143 FORMAT (///,12H LOOP NUMBER,I5)                                   A 3780
  144 FORMAT (2I10)                                                     A 3790
  145 FORMAT (20H0NDIV(I,1) NDIV(I,2))                                  A 3800
  146 FORMAT (20H0  JOIN(I,J,K) ARRAY)                                  A 3810
  147 FORMAT (4(I7,I3))                                                 A 3820
  148 FORMAT (20H0      XCOR       YCOR)                                A 3830
  149 FORMAT (2F10.3)                                                   A 3840
  150 FORMAT (30H0        NP       XORD       YORD)                    A 3850
  151 FORMAT (I10,2F10.3)                                               A 3860
  152 FORMAT (40H0  ELEM                                      NP )      A 3870
  153 FORMAT (4I9)                                                      A 3880
  154 FORMAT (20H1    NUMNP      NUMEL)                                 A 3890
  155 FORMAT (2I10)                                                     A 3900
  156 FORMAT (10H0   IPUNCH)                                            A 3910
  157 FORMAT (I10)                                                      A 3920
  158 FORMAT (20I5)                                                     A 3930
  159 FORMAT (1H0)                                                      A 3940
  160 FORMAT (I10)                                                      A 3950
```

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  161 FORMAT (10H1      NCON)                                          A 3960
  162 FORMAT (2I10)                                                    A 3970
  163 FORMAT (/, 22H OLD NUMBER NEW NUMBER,/)                          A 3980
C                                                                      A 3990
      END                                                              A 4000
```

SUBROUTINE SETUP

```
      SUBROUTINE SETUP (NUMNP,NUMEL,NCON,JT,IDIFF)                     A   10
      COMMON /BLK1/ JMEM(300),MEMJT(2000),JNT(300)                     A   20
      DIMENSION JT(2000)                                               A   30
C                                                                      A   40
C                                                                      A   50
      IDIFF=NUMNP                                                      A   60
C                                                                      A   70
      DO 101 J=1,NUMNP                                                 A   80
  101 JMEM(J)=0                                                        A   90
      DO 106 J=1,NUMEL                                                 A  100
         DO 105 I=1,4                                                  A  110
            JNTI=JT(NUMEL*(I-1)+J)                                     A  120
            IF (JNTI.EQ.0) GO TO 106                                   A  130
            JSUR=(JNTI-1)*NCON                                         A  140
C                                                                      A  150
            DO 104 II=1,4                                              A  160
               IF (II.EQ.I) GO TO 104                                  A  170
               JJT=JT(NUMEL*(II-1)+J)                                  A  180
               IF (JJT.EQ.0) GO TO 105                                 A  190
               MEM1=JMEM(JNTI)                                         A  200
               IF (MEM1.EQ.0) GO TO 103                                A  210
C                                                                      A  220
               DO 102 III=1,MEM1                                       A  230
                  IF (MEMJT(JSUR+III).EQ.JJT) GO TO 104                A  240
  102          CONTINUE                                                A  250
  103          JMEM(JNTI)=JMEM(JNTI)+1                                 A  260
               MEMJT(JSUB+JMEM(JNTI))=JJT                              A  270
               IF (IABS(JNTI-JJT).GT.IDIFF) IDIFF=IABS(JNTI-JJT)       A  280
  104       CONTINUE                                                   A  290
  105    CONTINUE                                                      A  300
  106 CONTINUE                                                         A  310
      RETURN                                                           A  320
C                                                                      A  330
      END                                                              A  340
```

SUBROUTINE OPTNUM

```
      SUBROUTINE OPTNUM (NUMNP,NUMEL,NCON,IDIFF)                       C   10
      COMMON /BLK1/ JMEM(300),MEMJT(2000),JNT(300)                     C   20
      DIMENSION JOINT(300), NEWJT(300)                                 C   30
C                                                                      C   40
C                                                                      C   50
      MINMAX=IDIFF                                                     C   60
      DO 107 IK=1,NUMNP                                                C   70
         DO 101 J=1,NUMNP                                              C   80
            JOINT(J)=0                                                 C   90
  101    NEWJT(J)=0                                                    C  100
         MAX=0                                                         C  110
         I=1                                                           C  120
         NEWJT(1)=IK                                                   C  130
         JOINT(IK)=1                                                   C  140
         K=1                                                           C  150
  102    K4=JMEM(NEWJT(I))                                             C  160
         IF (K4.EQ.0) GO TO 104                                        C  170
         JSUR=(NEWJT(I)-1)*NCON                                        C  180
C                                                                      C  190
         DO 103 JJ=1,K4                                                C  200
            K5=MEMJT(JSUR+JJ)                                          C  210
            IF (JOINT(K5).GT.0) GO TO 103                              C  220
            K=K+1                                                      C  230
            NEWJT(K)=K5                                                C  240
            JOINT(K5)=K                                                C  250
            NDIFF=IABS(I-K)                                            C  260
            IF (NDIFF.GE.MINMAX) GO TO 107                             C  270
            IF (NDIFF.GT.MAX) MAX=NDIFF                                C  280
  103    CONTINUE                                                      C  290
C                                                                      C  300
         IF (K.EQ.NUMNP) GO TO 105                                     C  310
  104    I=I+1                                                         C  320
         GO TO 102                                                     C  330
  105    MINMAX=MAX                                                    C  340
         DO 106 J=1,NUMNP                                              C  350
  106    JNT(J)=JOINT(J)                                               C  360
  107 CONTINUE                                                         C  370
C                                                                      C  380
      WRITE (6,108) MINMAX                                             C  390
C                                                                      C  400
C                                                                      C  410
      RETURN                                                           C  420
C                                                                      C  430
  108 FORMAT (//10X,20HREDUCED BAND-WIDTH =,I4//)                      C  440
C                                                                      C  450
      END                                                              C  460
```