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The Use of Galerkin Finite-Element Methods to Solve Mass-Transport Equations

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THE USE OF GALERKIN FINITE-ELEMENT METHODS TO SOLVE MASS-TRANSPORT EQUATIONS

By David B. Grove

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METRIC-ENGLISH EQUIVALENTS

Multiply English unit	*By*	*To obtain metric unit*
feet (ft)	0.3048	meters (m)
cubic feet per second (ft^3/s)	0.0283	cubic meters per second (m^3/s)

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ABSTRACT

The partial differential equation that describes the transport and reaction of chemical solutes in porous media was solved using the Galerkin finite-element technique. These finite elements were superimposed over finite-difference cells used to solve the flow equation. Both convection and flow due to hydraulic dispersion were considered. Linear and Hermite cubic approximations (basis functions) provided satisfactory results; however, the linear functions were found to be computationally more efficient for two-dimensional problems. Successive over relaxation (SOR) and iteration techniques using Tchebyschef polynomials were used to solve the sparce matrices generated using the linear and Hermite cubic functions, respectively. Comparisons of the finite-element methods to the finite-difference methods, and to analytical results, indicated that a high degree of accuracy may be obtained using the method outlined. The technique was applied to a field problem involving an aquifer contaminated with chloride, tritium, and strontium-90.

INTRODUCTION

It has become evident that our social and economic well-being is jeopardized by the ever-increasing pollution of our water resources. The hydrologic systems that control these resources do not act as separate entities, but as vast, complicated, interdependent systems. Due to the increasing stresses placed on surface-water resources, the public has become more aware of the vast amounts of high-quality water available underground in aquifers. As more is learned about these sources of water, both use and dependence upon them has increased. This use has both beneficial and detrimental aspects as it includes using the ground-water system for both sources of high-quality water and as reservoirs to dispose of unwanted aqueous wastes. This disposal practice coupled with the increasing withdrawal of water and the occasional influx of natural low-quality water, has in some instances rendered unfit previously usable ground-water supplies.

With recognition of these problems, Federal, State, and local agencies have enacted laws pertaining to the subsurface disposal of wastes and to the use of ground water. Enforcement of such laws and proper planning of ground-water use and subsurface waste-disposal practices necessitates a complete understanding of the ground-water systems and the effects of the chemical and physical stresses placed on them. In recent years considerable effort has been devoted towards developing techniques to compute the effects of various chemical and physical stresses on the ground-water system and the resultant change in water quality and quantity. The solution procedures for pollution simulation studies are termed "water-quality models." These techniques include simulation models, usually of a deterministic type, that may take the form of analytical expressions for simplified cases, or may involve the use of elaborate computer-oriented numerical techniques for the more complicated cases. The complicated nature of the mathematics defining the flow of pollutants through aquifer systems generally requires sophisticated numerical techniques to solve the equations. Some of the numerical techniques currently available have limited application because of their coarseness of approximation to the actual processes or are of such detail and complexity that their application to real problems is too difficult or impractical.

This report describes a numerical model that is rigorous in its solution to the equations yet simple enough that it may be used and understood by a knowledgeable ground-water hydrologist or engineer. The accuracy of the model is verified by various checks with known analytical solutions to simplified problems. The technique is also compared with results from a previously developed numerical technique for more involved systems. The value of this generalized numerical scheme is demonstrated by solving a ground-water contamination problem. The contamination problem includes the effects of transverse and longitudinal dispersion, and sink and source terms with rate and equilibrium-controlled chemical reactions for multidimensional mass-transport systems.

I would like to acknowledge John Robertson, Research Hydrologist, who furnished the results of his field study at the Idaho National Engineering Laboratory, that were used to provide the field test of the model, and Dr. Thomas Manteuffel, Professor of Mathematics, Emory University, who provided the results of his then unpublished Ph. D. thesis to solve a difficult problem involving large, sparce, unsymmetric matrix systems.

REVIEW OF THE LITERATURE

This section consists of three separate parts that are as follows: The development of equations pertaining to the transport of solute, the analytical solutions of some of these equations, and the numerical solutions of these equations encompassing both finite-difference and finite-element methods. Experimental studies and case histories are included within each respective solution technique. The literature in the field of mass transport is great and this review includes only those that are specific to this study. The references are limited to the past 4 or 5 years as the majority of the work previous to this time is well documented in these references.

Prior to the past several years the prediction of the quality of water during its movement through porous media was limited to laboratory studies, controlled industrial processes, or pure theory. This was due to a lack of ability to define accurately multidimensional flow fields, an incomplete mathematical model of solute transport, inadequate numerical schemes to solve the equations, incomplete descriptions of the relevent chemical reactions taking place, and a much lower interest in solving such problems for actual field situations.

During the last 4 to 5 years, however, models and modeling techniques have developed at an accelerated rate. The usual water-quality model development procedure has been to simplify the general multidimensional transient equations describing mass transport and reactions to one-dimensional situations that can be simulated by controlled laboratory experiments or can be solved in a closed analytical form. The simplifying assumptions are then relaxed and the general model applied to more complex situations. Two-dimensional models for solute transport without chemical reactions but including terms to describe nonideal (plug) flow, which we term "dispersion," and the existence of sources and sinks within the system were then developed. Investigators refined these models to include the capability to predict and verify chemical reactions for selective field situations. Solution techniques for the equations of solute transport include finite-difference methods, method of characteristics, and finite-element methods that encompass variational and weighted residual techniques. These methods will be reviewed in more detail to provide a proper framework for the development of the Galerkin, finite-element techniques.

Development of the equations

The equations of mass transport with chemical reactions have been well documented by physicists, chemists, and chemical engineers, as is evidenced by the text of Bird, Stewart, and Lightfoot (1966) and Aris (1969). Bredehoeft and Pinder (1973), also Rendell and Sanada (1970), expanded on these basic equations and coupled them with the hydraulic flow equations to present a unified picture of mass transport with or without chemical reactions during flow through saturated porous media.

The flow equation

The equation of motion for the flow of ground water has been derived in considerable detail by a variety of workers. Longwell (1966) and Bredehoeft and Pinder (1973) present rather complete derivations of the equation. Bredehoeft and Pinder (1973) described ground-water flow by the following equation:

$$\nabla \cdot \left[\rho \frac{\bar{\bar{k}}}{\mu} \cdot (\Delta p - \rho \bar{g}) \right] + \sum_{i=1}^{r} W_i = \rho \alpha \frac{\partial p}{\partial t}$$

$$+ \rho_o \varepsilon \beta \frac{\partial p}{\partial t} + \frac{\varepsilon}{V_o} \sum_{j=1}^{n} \frac{\partial m_j}{\partial t} \qquad (1)$$

where

∇ = vector operator

ρ = fluid density, ML^{-3}

$\bar{\bar{k}}$ = intrinsic permeability, L^{+2}

μ = dynamic viscosity, $ML^{-1}T^{-1}$

$\bar{g}$ = gravitational acceleration, LT^{-2}

Q_i = source (+) or sink (-) L^3T^{-1}

$$W_i(x,y,z) = \sum_{j=1}^{r} Q_i(x_j,y_j,z_j)\ \delta\ (x-x_j)\ \delta\ (y-y_j)\ \delta\ (z-z_j)$$

r = number of sources and sinks

α = compressibility of the medium, $M^{-1}LT^{+2}$

ε = effective porosity of the medium, L^o

δ = Dirac delta function

β_ρ = compressibility coefficient of the fluid, $LM^{-1}T^2$

V_o = reference volume of the fluid, L^3

m_i = mass of the i-th species in the reference volume V_o, M

n = total number of species in the system

Implicit in the derivation of the flow equation is Darcy's Law, which relates specific discharge to hydraulic gradient.

$$\bar{q} = -\frac{\bar{\bar{k}}}{\mu} \cdot (\nabla p - \rho \bar{g}) \tag{2}$$

where $\bar{q}$ is the specific discharge of the fluid, LT^{-1}. The hydraulic flow equation is a mathematical description of the hydraulic potential of the aquifer system. Equation 1 can be simplified by assuming constant fluid density (Bredehoeft and Pinder, 1973), and written in two dimensions (areal) as

$$S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(T_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy} \frac{\partial h}{\partial y}\right)$$

$$- W(x,y,t) \tag{3}$$

where

S = aquifer storage coefficient, L^o

h = hydraulic head, L

T_{xx} = transmissivity of the aquifer in the x direction, L^2T^{-1}

T_{yy} = transmissivity of the aquifer in the y direction, L^2T^{-1}.

Equation 2 is a general form of Darcy's Law for an anisotropic porous media. The permeability axis can be orientated in such a direction so only the main components of the permeability tensor appear. When this is possible and all of the pressure terms appear in the hydraulic gradient, specific discharge for flow in the x direction is

$$q_x = -k_x \frac{\partial h}{\partial x} \tag{4}$$

A similar equation may be written for the y-direction. The average interstitial fluid velocity, as will be used in the mass-transport equation, is defined as the specific discharge divided by porosity and is given by

$$v_x = -\frac{k_x}{\varepsilon} \frac{\partial h}{\partial x} \tag{5}$$

where

v_x = average interstitial velocity in the x direction, LT^{-1}

ε = porosity, L^o.

The mass-transport equation

The mass-transport equation for solute species i as given by Bredehoeft and Pinder (1973) is

$$\varepsilon\rho_i\alpha\frac{\partial p}{\partial t} + \frac{\partial}{\partial t}(\varepsilon\rho_i) = \nabla\varepsilon\rho\bar{\bar{D}}_i\nabla\left(\frac{\rho_i}{\rho}\right)$$

$$- \nabla\rho_i\bar{q} + \sum_{k=1}^{s} R_{ik} + W_i\rho_i^* \qquad (6)$$

where

ρ_i = density of species i, ML^{-3}

$\bar{\bar{D}}_i$ = hydrodynamic dispersion coefficient of species i, L^2T^{-1}

R_{ik} = rate of production of species i in reaction k, $ML^{-3}T^{-1}$

s = number of reactions taking place in system

ρ_i^* = density of sink or source solution, ML^{-3}

The mass-transport equation as given by equation 6 can be simplified and written in two dimensions (Bredehoeft and Pinder, 1973; Reddell and Sunada, 1970) as equation 7.

$$\frac{\partial c_i}{\partial t} = - v_x\frac{\partial c_i}{\partial x} - v_y\frac{\partial c_i}{\partial y} + \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c_i}{\partial y}\right)$$

$$+ \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{xy}\frac{\partial c_i}{\partial y}\right) - \left(c_{wi} - c_i\right)\frac{W_i}{\varepsilon} \qquad (7)$$

$$+ \sum_{k=1}^{s} R_{ik}$$

where

c_i = mass concentration of species i, ML^{-3}

c_{wi} = mass concentration of species in the well, ML^{-3}

and the subscripts x and y define the direction of interest for the respective variables.

This equation is simplified from that given by Bredehoeft and Pinder (1973), as it assumes that the time derivative of pressure in the transport equation is small compared to the other terms and may be neglected. This is actually a good assumption as steady state flow does exist for many problems, and for transient conditions this assumption introduces little error. Constant fluid density, as assumed for equation 3, is also implicit in equation 7, as the density is assumed to be unaffected by changes in concentration.

Equations 3, 5, and 7 represent, for isothermal systems, all that is necessary to adequately approximate conditions in most systems. Equation 3 is the flow equation with hydraulic head calculated as the dependent variable for the space and time fields of interest. Equation 7, the "transport equation," is coupled to equation 3 by Darcy's Law (equation 5), which relates ground-water velocity to hydraulic head gradient.

The mass transport equation consists of four terms; the mass accumulation term on the left-hand side of the equation, the convective fluxes, the dispersion flux terms, the sink/source term, and the chemical reaction term on the right-hand side of the equation. These terms and the parameters that comprise them will be discussed in more detail in the section on the mass-transport equation.

Analytical solutions

In many cases equation (7) can be simplified to the point where analytical solutions are available. Solutions for some of these simpler differential equations representing mass transport are important for several reasons. Several of the contamination problems are well represented by one-dimensional equations, and in this case simple analytical solutions can be used to predict the extent and concentration of contaminations. A second reason is that many complicated multidimensional models can be simplified and their accuracy or precision checked with the aid of these simple one-dimensional equations.

Perhaps the equation most widely used to analyze the effects of convection and dispersion in a porous media is the one-dimensional equation with unidirectional flow. This equation results through simplification of equation 7 and is presented with boundary conditions as given by Ogata and Banks (1961)

$$\frac{\partial c}{\partial t} = - v \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} \qquad (8)$$

$c = c_o$ for $x = 0$, $t \geq 0$

$c = 0$ $x \to \infty$, $t \geq 0$

$c = 0$ $x > 0$, $t = 0$

These boundary conditions describe the physical situation as illustrated in figure 1. A slug of fluid with concentration c_o is injected into a column at $x = 0$ and at time = 0. This slug of fluid is then convected and dispersed in the longitudinal direction. The column is assumed of infinite extent and the solution is for the relative concentration of the injected fluid at any time t at location x. Ogata and Banks solution to this equation is given as follows:

$$\frac{c}{c_o} = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x-vt}{\sqrt{4Dt}}\right) + \exp\left(\frac{vx}{D}\right)\operatorname{erfc}\left(\frac{x+vt}{\sqrt{4Dt}}\right)\right] \tag{9}$$

Equation 9 describes the process of dispersion in a porous media when the dispersion coefficient is relatively small and when one is interested in concentration profiles in the porous media and not at the exit of the column.

Brenner (1962) analyzed the same physical situation; however, he defined the boundary conditions at the inlet and outlet of the column in a more rigorous and specific manner. Brenner assumed the following boundary conditions:

$$D\frac{\partial c}{\partial x} = -v\,(c - c_o) \quad \text{for } x = D,\ t \geq 0$$

$$\frac{\partial c}{\partial x} = 0 \quad \text{for } x = L,\ t \geq 0$$

which define flux conditions at the inlet and outlet of the column. Brenner's solution is more complicated and is given for the relative concentration at the exit of a column of length L:

$$\frac{c}{c_o} = \exp\,[P(2-T)] \sum_{k=1}^{\infty} \frac{\lambda_k \sin\,(2\lambda_k)}{(\lambda^2{}_k + P^2 + P)} \exp\left(-\lambda^2{}_k T/P\right) \tag{10}$$

where

$T = vt/L$

$P = vL/4D$

λ_n = the positive roots ($k = 1, 2, \ldots, n$) taken in order of increasing magnitude of the equation, and where,

$$\tan 2\lambda = \frac{2\lambda P}{\lambda^2 - P^2} \tag{11}$$

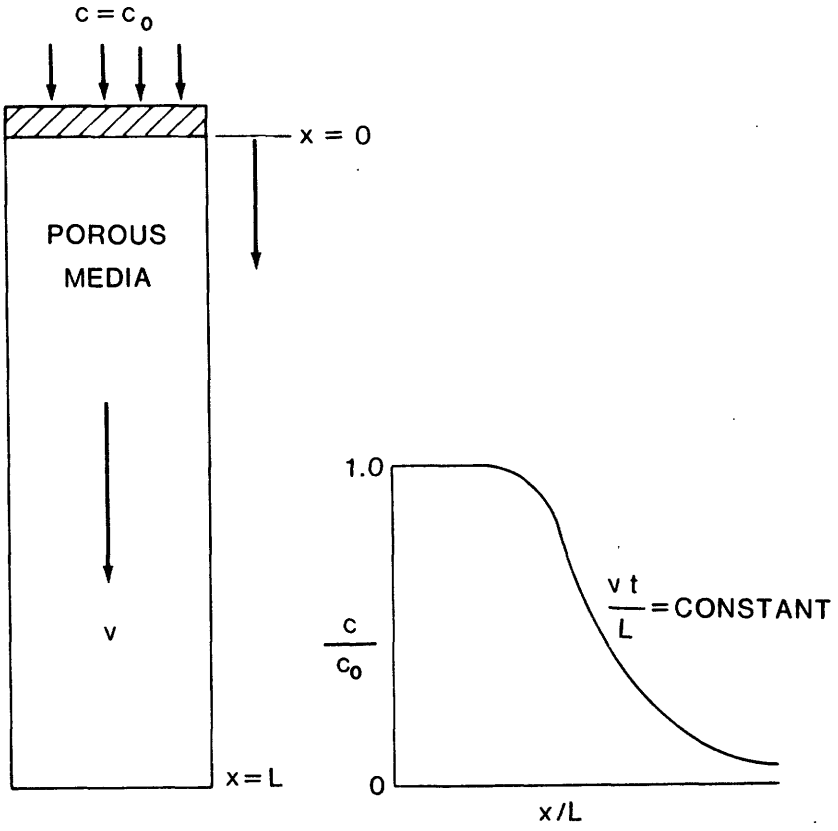


Figure 1.--*Longitudinal dispersion in a column.*

Brenner (1962) included a tabulation of concentrations at the column exit for various values of P.

Numerical solutions

Finite-difference methods

Perhaps the commonly used numerical technique used to solve both linear and nonlinear differential equations describing mass transport is the finite-difference method. Finite-difference techniques, (if not careful) display numerical difficulties when applied to these particular types of equations. These problems can perhaps best be explained in the context of the following one-dimensional differential equation as illustrated by Keller (1967):

$$\frac{\partial u}{\partial t} = a(x,t)\frac{\partial^2 u}{\partial x^2} + 2b(x,t)\frac{\partial u}{\partial x} - c(x,t)u + d(x,t) \tag{12}$$

A typical finite-difference form to this equation, when variables are centered in space, can be written as follows:

$$u_j^{n+1} - u_j^n = \lambda a^{n+\Theta}\left(u_{j+1}^{n+1} - 2u_j^{n+\Theta} + u_{j-1}^{n+\Theta}\right) + \Delta x\lambda b^{n+\Theta}\left(u_{j+1}^{n+\Theta} - u_{j-1}^{n+\Theta}\right)$$

$$- \Delta t c_j^{n+\Theta} u_j^{n+\Theta} + \Delta t d_j^{n+\Theta} \tag{13}$$

where

$u^{n+\Theta} = \Theta\, u_j^{n+1} + (1-\Theta)u_j^n$

Θ = time approximation

$\lambda = \Delta t/(\Delta x)^2$

n = time superscript

j = distance subscript

Values of Θ may be 0, 1/2, or 1. The 0 denotes an explicit in time approximation; the 1/2, a centered in time or Crank Nicolson time approximation; and Θ equals 1, a fully implicit or backwards in time approximation.

These typical finite-difference forms result in the following system of linear equations

$$\alpha_j\, u_{j-1}^{n+1} + \beta_j u_j^{n+1} + \gamma_j u_{j+1}^{n+1} = S_j^n \tag{14}$$

As with most finite-difference equations, stable solutions occur only with the proper choice of time and space-increment sizes. The following conditions are given by Keller (1967) as sufficient to provide stable nonoscillatory solutions to equation 13:

$$1 + \theta\Delta tc(x,t) > 0 \qquad (a)$$

$$a(x,t)\Delta x|b(x,t)| \geq 0 \qquad (b) \qquad (15)$$

$$1 - (1-\theta)\,[2\lambda a(x,t) + \Delta tc(x,t)] \geq 0 \qquad (c)$$

Condition 15a is usually not a problem as values of concentration are normally positive. Condition 15b results in numerical oscillation if not met, and although damped, it may be so large in magnitude to preclude adequate numerical values. For fixed values of a and b, condition 15b requires a small value of the space increment. Condition 15c is met for all fully implicit methods. One must also note that these are "sufficient" and not necessary conditions for stability, and in many cases when θ is equal to 1/2, stable solutions result even if condition 15c is not satisfied.

The conditions where finite-difference solutions can be used to solve the differential equations defining mass transport through porous media have been identified. However, the technique that gives stable solutions may result in an additional error caused by the manner in differencing the time and space derivatives. This error is called numerical diffusion as its form is identical to the second-order diffusion term in the equation. For equation 8, the one-dimensional equation describing convection-dispersion, Lantz (1970a; 1970b) calculated the magnitude of this numerical diffusion term for various types of spatial and time increments. Table 1 summarizes the results of Lantz's study. Some authors (for example, Harlow and Amsden, 1970) reasoned that the total diffusion term in the equation, both real and numerical, must be positive. Table 1 then indicates that when spatial properties are differenced centrally and time is differenced explicitly, the dispersion coefficient in the equation must be larger than the numerical diffusion term or a negative result appears and unstable solutions result. Table 1 also shows that a spatial central difference and a time Crank-Nicolson difference gives no numerical diffusion error. However, this does not rectify the stability condition given in 15b where the choice of a large spacial increment may cause oscillation in the computed concentration profile. It appears that for all cases small space increments are necessary for adequate solutions of equations with small dispersion coefficients. This does not normally present a problem for one-dimensional equations; however, multidimensional equations result in large numbers of nodes that produce matrices too large to be solved efficiently with present-day computers.

Peaceman and Rachford (1962) presented a finite-difference scheme to solve the two-dimensional transport equation. They illustrated the oscillation problem, caused by small dispersion coefficients, for the one-dimensional case and presented a "transfer of overshoot or undershoot" correction technique. Shamir and Harleman (1967) studied a steady-state flow situation and solved the mass-transport equation in terms of streamlines and velocity potentials. Since the velocity is parallel to the streamline, one-dimensional flow could be assumed and the dispersion tensor cross-product terms omitted. Unfortunately both of these approaches have restrictions. The "transfer of overshoot" method of Peaceman and Rachford is not rigorous and the use of streamlines assumes steady-state flow conditions and unrealistic one-dimensional flow.

Table 1--*Numerical diffusion errors caused by various space and time differencing of the convective term in the 1-D mass-transport equation*

[BD, backward difference; CD, central difference, C-N, Crank-Nicolson]

Difference form		Error (second order) x $\frac{\partial^2 c}{\partial x^2}$
Spacial	Time	
BD	Explicit, Θ=0	$(v\Delta x - v^2\Delta t)/2$
CD	Explicit	$-v^2\Delta t/2$
BD	Implicit, Θ=1	$(v\Delta x + v^2\Delta t)/2$
CD	Implicit	$v^2\Delta t/2$
BD	C-N, Θ=1/2	$v\Delta x/2$
CD	C-N	0

Method of characteristics

Gardner and others (1964) used a method of characteristics (MOC) to solve the mass-transport equation. They essentially modified the MOC method to include a point-tracking technique by which particles were given various concentrations and allowed to move with the velocity of water to new points for various time increments. Concentrations were averaged over the various grid domains and the dispersion process calculated by an explicit finite-difference method. Reddell and Sunada (1970) and Bredehoeft and Pinder (1973) expanded the one-dimensional case of Garner's to two dimensions. Pinder and Cooper (1970), as well as Reddell and Sunada (1970), utilized the characteristics method to include density dependence and solved a salt-water encroachment problem.

The method and the computer program as developed by Bredehoeft and Pinder (1973) have been extensively used within the U.S. Geological Survey to solve field problems involving contamination. Several such studies are as follows: In Georgia, Bredehoeft and Pinder (1973) investigated a contamination problem where saline water upwelled into a fresh-water aquifer and computed the effects of discharge or barrier wells to limit this concentration spread. Hughes and Robson (1973) investigated contamination from sewage lagoons and industrial cleaning areas and predicted the results of various ground-water quality containment practices. Konikow and Bredehoeft (1974) investigated the effects of

irrigation and return flow on water quality in the ground-water system and in the adjacent river. Perhaps the best documented use of the method of characteristics to solve the mass-transport equation has been the application of Robertson and Barraclough (1973) at the National Reactor Testing Station in Idaho Falls, Idaho. They modeled the movement of injected pollutants into a basaltic aquifer and determined the concentration profile for a period of 20 years. Robertson (1974) modified the mass-transport equations to include the chemical reaction terms that accounted for ion exchange and radioactive decay.

These studies demonstrated the worth of the method of characteristics for modeling two-dimensional mass transport but they also showed it to be cumbersome, expensive, and lacking in mathematical rigor. This latter point is demonstrated by the use of experience in the placement and number of particles used in MOC. The method of characteristics is perhaps the best technique for hyperbolic equations. The ability to set the dispersion coefficient equal to zero and to model pure convective flow is a distinct advantage for this method. Most processes, however, do involve nonideal flow, which is characterized by the hydrodynamic dispersion. Simpler numerical techniques that will apply under these cases should be considered.

Finite-element methods

Finite-element methods involve integration of some function pertaining to the differential equation over some prescribed element or area. Integration methods, relationship between function and differential equation, and definition of the element over which integration proceeds, all serve to characterize different methods. Most textbooks separate the finite-element technique into variational techniques and weighted-residual techniques. The variational technique will be discussed first.

Variational techniques

The use of variational calculus to solve partial differential equations that describe transport processes has recently received widespread attention (Forray, 1968; Schechter, 1967). The coupling of finite elements and variational calculus has led to a numerical technique that has great promise when the variational principles apply. The flow equation (3) has been programmed and solved for some time using this method. Remson, Hornberger, and Molz's text (1971) on numerical procedures for these types of aquifer equations discusses at some length the techniques and previous work done in this field. Guymon and others (1970) perhaps first solved the multidimensional convection-diffusion equations using finite-element variational methods. Guyman's work was expanded by Nalluswami (1971), who improved the numerical techniques and took into account the tensoral properties of the dispersion coefficient. A recent paper by Smith, Farroday, and O'Conner (1973) compares the variational finite-element technique with the soon-to-be-discussed Galerkin finite-element technique. The overall concensus of this paper was, unless a definite-variational principal exists so that the solution procedures would be identical, the Galerkin finite-element technique was superior in its efficiency and accuracy in solving the mass-transport equation. All the aforementioned studies of the mass-transport equation were compared with analytical cases with no application made to a field problem.

Weighted-residual techniques

Weighted-residual techniques are defined by the method used to weight the residual formed by an approximation to the partial differential equation and the method used to calculate the approximate solutions. Although there are several weighted-residual methods, Finlayson and Scriven (1965) found the Galerkin method best for mass-transport equations. The mathematics associated with the finite-element use of the Galerkin weighted-residual method will be developed in the following section. Price, Cavendish, and Varga (1968) first showed the superiority of the Galerkin finite-element method over the standard finite-difference method to solve the one-dimensional mass-transport equation. Cavendish, Price, and Varga (1969) utilized this technique to solve nonlinear and multidimensional flow equations. They concluded that for linear equations this method was superior to standard finite-difference methods.

Pinder (1973) used a Galerkin finite-element technique with the use of isoparametric quadralateral elements to solve a ground-water contamination problem on Long Island, N.Y. In this case, elements could take on a variety of configurations and by a mapping procedure be reduced to rectangles. The resulting set of linear equations were solved by a direct matrix technique. This application did not include the introduction of point sources or sinks (as wells), and the contaminant was conservative in that chemical reactions involving the solute were absent. This technique requires the choice of specific approximating functions somewhat limiting its applicability.

THE MASS-TRANSPORT EQUATION

The equations that will be used to define the concentrations of induced chemical species are the flow equation (3), Darcy's Law (5), and the transport equation (7), respectively. As mentioned previously, the transport equation consists of four main terms on the right-hand side that account for changes of concentration. These are the convective flux, the dispersive flux, physical sink/source terms, and chemical reaction terms. These terms and the parameters that make them up will now be discussed in more detail.

Convective and dispersive fluxes

The convective flux is defined as that mass transport caused by the bulk movement of the fluid. The velocities are derived from the potential (flow) equation using Darcy's Law. The dispersive flux term is a vector quantity and, as such, deserves more explanation. Scheidegger (1961) and Bear (1972) point out that the dispersion coefficient is then a tensor and should have 81 components for a three-dimensional case, but they are able through the use of symmetry to reduce this number to 32 individual components. They are able, for an isotropic media, to reduce the number of components of the tensor to nine for a three-dimensional case and four for the two-dimensional case.

The general form of the dispersion tensor is given by Scheidegger (1961) as

$$D_{kl} = \sum_{i=1}^{2} \sum_{j=1}^{2} a_{ijkl} v_i v_j / |V| \qquad \text{for } k = 1,2 \qquad (16)$$

where

$1 = x$
$2 = y$

and

$$a_{ijkl} = \alpha_L \delta_{ij} \delta_{kl} + \frac{(\alpha_L - \alpha_T)}{2} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \tag{17}$$

where

δ_{ij} = dirac delta function = 1, i=j
= 0, i≠j

α_L = longitudinal dispersivity, L

α_T = transverse dispersivity, L

The longitudinal and transverse dispersivities are sometimes referred to as characteristic lengths with their magnitude a measure of the total dispersion.

The four dispersion coefficients of two-dimensional flow can now be written as

$$D_{xx} = \alpha_L v_x^2 / |V| + \alpha_T v_y^2 / |V|$$

$$D_{yy} = \alpha_L v_y^2 / |V| + \alpha_T v_x^2 / |V|$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) v_x v_y / |V| \tag{18}$$

where

$$|V| = \sqrt{v_x^2 + v_y^2}$$

Sinks and sources

In the mass-transport equation, there are a variety of sink and source terms that must be considered. The most obvious ones are inputs or outputs in the system caused by wells or leakage through the aquifer. Chemical reactions are another means to increase or decrease the concentrations of solute species. After discussing point sources, two of the most frequently occurring reactions will be discussed in detail.

Point and distributed terms

Concentration changes caused by the convective flow of solutes in or out of an aquifer can occur through wells or areas normal to the flow field. The term representing such effects in equation 7 is

$$(c_{iw}c_i)\frac{W_i}{\varepsilon} = \sum_{i=1}^{r} Q_i(x_i,y_i)(c-c_{iw})\delta(x-x_i)\delta(y-y_i) \qquad (19)$$

where c_{iw} is the concentration of the fluid recharging or discharging from the system through the well. The term $c_{iw}-c$ is equal to zero for a pumping well as c_{iw} equals c_i. The dirac delta function assures values for the term only at nodal points where wells are present.

Chemical reactions

Two principal chemical reactions that often occur in contamination problems are equilibrium-controlled ion exchange reactions with a linear adsorption isotherm and irreversible first-order rate reactions. The mathematics that describe these reactions are linear and thus allow the use of simpler numerical solution techniques. The addition of linear terms to a differential equation, in most cases, requires no additional mathematical analysis. The use, for example, of a zero-order reaction would cause no problem in analytical or numerical analysis.

Ion exchange

A typical such exchange reaction might be as follows (Bolt, 1967; Helfferich, 1962)

$$b\,\bar{c}_1 + a\,c_2 \rightleftharpoons a\,\bar{c}_2 + b\,c_1 \qquad (20)$$

where 1 and 2 are chemical exchanging species with a and b valences, respectively.

The adsorbed species is given as $\bar{c}$ and the dissolved species as c. A selectivity coefficient may be used to relate the concentration of products and reactants at equilibrium:

$$K_s = \frac{(\bar{c}_2)^a(c_1)^b}{(\bar{c}_1)^b(c_2)^a} \qquad (21)$$

where K_s is the ion exchange selectivity coefficient.

Equation 21, when incorporated into the mass-transport equation, results in nonlinear terms. One particular situation that often occurs results in a simplified equation, and is described as follows: When the exchanging ion is very low in concentration relative to the other ions, then exchange process will not materially effect the concentration of this ion, either in solution or adsorbed on the matrix. The adsorbed phase of the major ion is then nearly equal to the cation exchange capacity (CEC), and the solution phase of the major ion equals the total concentration (C_o). Equation 21 can then be rewritten as,

$$K = \frac{(\bar{c}_2)^a (C_o)^b}{(CEC)(c_2)^a} \tag{22}$$

or

$$K_d = \frac{\bar{c}_2}{c_2} = \left[\frac{K_s (CEC)^b}{(C_o)^b}\right]^{1/a} \tag{23}$$

where K_d = ion exchange distribution coefficient.

Equation 23 postulates a linear relationship between the adsorbed species and the solute species where the slope of the equilibrium ion-exchange isotherm is the distribution coefficient. Equation 23 thus provides the relationship between the adsorbed species and dissolved species necessary to solve the mass-transport equation.

Rate reactions

The subsurface disposal of radioactive products is an example where a first-order irreversible rate reaction occurs. This reaction is the radioactive decay of the species, adsorbed or in solution. The rate constant can be derived in the following manner. The disappearance of a species by a first-order irreversible reaction is given by the equation

$$\frac{dc}{dt} = - kc \tag{24}$$

where k is the rate constant, T^{-1}. This equation can be integrated with the limits chosen as the time necessary for the initial concentration to decrease by one-half

$$\int_{c_o}^{c_o/2} \frac{dc}{c} = -k \int_0^{t_{\frac{1}{2}}} dt \tag{25}$$

where c_o = initial concentration, ML^{-3}

$t_{\frac{1}{2}}$ = half life of species, T

The equation is integrated and solved for k to obtain

$$K = \frac{0.693}{t_{\frac{1}{2}}} \tag{26}$$

The rate constant can now be calculated as half-lifes of most radioactive species are known.

The chemical reactions terms can now be incorporated into the mass-transport equation in the following manner: Assume the transport of a chemical species is disappearing by a first-order irreversible rate reaction and is being exchanged reversibly by an equilibrium-controlled process in which the exchange isotherm is linear. The equation describing this reaction in one dimension is

$$\frac{\partial c}{\partial t} + \frac{\rho_b}{\varepsilon}\frac{\partial \bar{c}}{\partial t} = - v\frac{\partial c}{\partial x} + D\frac{\partial^2 c}{\partial x^2} - k\left(c + \frac{\bar{c}\rho_b}{\varepsilon}\right) \tag{27}$$

where ρ_b = bulk density of the solid matrix, ML^{-3},

c = dissolved species concentration,

$\bar{c}$ = adsorbed species concentration.

Equation 23 gives the relationship between c and $\bar{c}$ and upon differentiation and substitution into equation 27, gives

$$\frac{\partial c}{\partial t}\left(1 + \frac{K_d\rho_b}{\varepsilon}\right) = - v\frac{\partial c}{\partial x} + D\frac{\partial^2 c}{\partial x^2} - kc\left(1 + \frac{K_d\rho_b}{\varepsilon}\right) \tag{28}$$

The retardation factor R_f is defined as

$$R_f = 1 + K_d\rho_b/\varepsilon \tag{29}$$

Equation 28 is divided by this retardation factor and the dispersion coefficient written proportional to a dispersivity term α_L to obtain

$$\frac{\partial c}{\partial t} = - \frac{v}{R_f}\frac{\partial c}{\partial x} + \frac{\alpha_L v}{R_f}\frac{\partial^2 c}{\partial x^2} - kc \tag{30}$$

The retardation factor thus describes the average amount of retardation in the flow of the solute species relative to the average interstitial velocity of water. This reduced velocity caused by adsorption is an important safety feature that prevents excessive movement of possibly harmful pollutants.

DEVELOPMENT OF THE GALERKIN FINITE-ELEMENT TECHNIQUE

The Galerkin technique is one of the weighted-residual methods discussed in its classical form by numerous authors (Crandall, 1956; Snyder and others, 1964; Finalyson, 1969 and 1972). It is shown to be the most efficient of these methods by Finalyson and Scriven (1965) for the solution of mass-transport equations. The Galerkin method is an old numerical technique, classically used to solve differential equations not ameanable to analytical techniques. Recent advance in computing techniques popularize this particular weighted-residual method by coupling it with the finite-element technique (see literature review section). The theoretical development of the technique by Douglas and Dupont (1970) lends strong basis for the use of this particular technique for the solution of mass-transport equations.

Theory

The principle of the Galerkin finite-element method is to first choose a set of functions discretized in space but continuous in time to approximate the solution of the differential equation. This set of approximating functions contains time-dependent coefficients and basis functions that are real valued and piecewise continuously differentiable over the interval of interest. If $L[c(t,x,y,z)]$ is the differential operator this series approximation is written as

$$c_\infty (t,x,y,z) = \sum_{i=1}^{\infty} c_i(t)v_i(x,y,z) \tag{31}$$

where c_∞ = approximate solution to the differential equation $L[c]=0$,

c_i = coefficient in the approximating function,

v_i = basis functions.

Since a finite number of coefficients must be evaluated, an nth order approximation to the solution results. This approximation is written

$$c_n(t,x,y,z) = \sum_{i=1}^{n} c_i(t)v_i(x,y,z) \tag{32}$$

where c_n = approximation to the solution for n terms. The closeness of this approximation, c_n, to the real solution, c, depends upon three criteria; (1) care in chosing proper basis functions; (2) the number of terms n in the series, and (3) the method used to evaluate the coefficients c_i. It is this third criteria, that of choosing the best method to evaluate these unknown coefficients, that separates the Galerkin method from the other weighted-residual methods. Weighted-residual methods use the concept of a residual, R, in their development. This residual is formed by substituting into the differential equation the previously mentioned series approximation for the dependent variable thus

$$L\left[c_\infty(t,x,y,z)\right] \approx L\left[c_n(t,x,y,z)\right]$$

$$= L\left[\sum_{i=1}^{n} c_i(t)v_i(x,y,z)\right] = R \qquad (33)$$

where L = the differential operator,
R = the residual.

The residual vanishes in the entire domain of interest or is identically equal to zero for a true solution to the equation. In general, a true solution will not result, and the residual will not be equal to zero. Galerkin's contribution to the weighted-residual methods is how to weight the residual in an optimum manner allowing the approximation to be accurate. Galerkin chose this weighting function identical to the approximating fuctions (basis functions) used in the original approximation and set this weighted average equal to zero. The weighted average of the residual can be defined and set equal to zero as follows:

$$\frac{\int_{dV} Rv_k(x,y,z)dV}{\int_{dV} v_k(x,y,z)dV} = 0 \text{ for } k = 1, 2, \ldots, n \qquad (34)$$

where v_k = weighting function,
R = residual.

Equations 33 and 34 can be combined to give

$$\int_{dV} L\left[\sum_{i=1}^{n} c_i(t)v_i(x,y,z)\right] v_k(x,y,z)dV = 0 \text{ for } k = 1, 2, \ldots, n \qquad (35)$$

When the series approximation, equation 32, is substituted into the differential equation L[c]=0, the approximation may have to be differentiated several times as the equation warrants. The differential equation may contain second-order derivatives and unless the basis functions can be differentiated twice, a trivial solution occurs. This problem can be rectified by integrating all second derivatives by parts. Simple integration by parts is defined for the variables u and v as

$$\int_a^b udv = uv\Big|_a^b - \int_a^b vdu \qquad (36)$$

This technique can be applied to multiple integrals as well.

After integration of equation 35, a set of n linear differential equations with the following form results:

$$[\alpha]\,\frac{\overline{dc_i}}{dt} + [\beta]\,\overline{c}_i + [\lambda] = 0 \tag{37}$$

where $[\alpha]$, $[\beta]$, and $[\lambda]$ are coefficient matrices resulting from the Galerkin integration, $\frac{\overline{dc_i}}{dt}$ and $\overline{c}_i$ are column vectors representing the unknown coefficients. This set of differential equations is then finite differenced with respect to time and the resulting set of linear algebraic equations solved by appropriate techniques, some of which will be discussed later.

Basis functions

Basis functions are usually chosen so that they have analytical properties that conform to the equation, boundary conditions, or result in simplified equations for ease of computation during the analysis process. The basis functions are usually defined over a limited number of finite elements. That is, they have values at element edges or intersections (nodes) of 0 or 1, respectively. Also they are usually easily integrated by some numerical or analytical technique. Simple polynomials are often used. Two common sets of basis functions are linear and cubic polynomials.

A linear set of basis functions w_i for one dimension is described over the preselected intervals as follows (Price and others, 1968; Doherty, written comm., 1972).

$$w_i(x) = \begin{cases} (x-(i-1)h)/h; & (i-1)h \le x < ih \\ ((i+1)h-x)/h; & \text{for } ih \le x \le (i+1)h \\ 0 & \text{otherwise} \end{cases} \tag{38}$$

These particular basis functions form roof or shingle-type straight-line segments over the interval of interest. Hence, they are given the name linear or chapeau basis functions. Figure 2 shows these basis functions over one-dimensional elements of length h. At the node points, each basis function has a value of one and all other basis functions have a value of zero. Each basis function is overlain by the two adjacent basis functions. Integration for a basis function w_k is thus required only over the area of three basis functions, thus, eliminating integration over the entire interval. This can be represented mathematically as

$$w_i(x_j) = \delta_{ij} \tag{38a}$$

$$\int_0^L Rw_k\,dx = \int_{x_{k-1}}^{x_k} Rw_k\,dx + \int_{x_k}^{x_{k+1}} Rw_k\,dx = 0 \tag{38b}$$

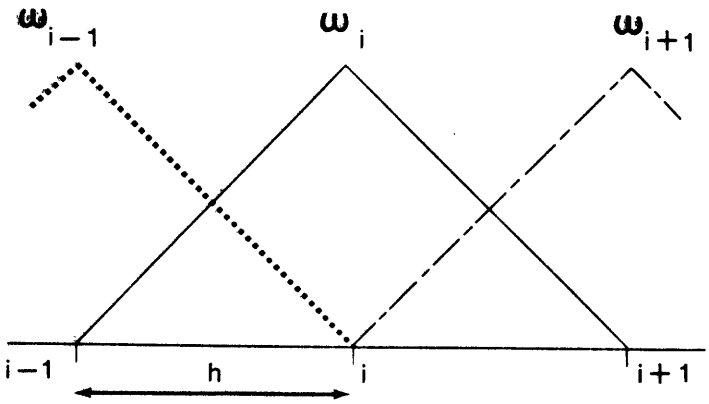


Figure 2.--*Plot of Chapeau basis functions with grid spacing h.*

The use of linear basis functions in linear one-dimensional problems results in a set of linear equations with three unknowns in each equation. The matrix associated with these equations is tridiagonal and therefore simple computional methods can be used for solution. The method is second-order accurate with respect to space, as are space-centered finite-difference equations, but has been shown (Price and others, 1968) to offer advantages in the prevention of solution oscillations not afforded by finite-difference techniques. Oscillations do occur, however, as element intervals become larger. The use of linear functions does not allow the user to obtain derivatives of the final solution at the node points, since derivatives of the basis functions are discontinuous at the nodes.

Another basis function commonly used is the Hermite cubic function. Figure 3 shows these basis functions over elements of length h. It is composed of two cubic polynomials that offer several advantages not available with the linear function. This particular set of functions is also defined over two elements (for one-dimensional problems), or three nodes. One polynomial has a value of zero at each end point and a value of one at the center. Slopes are zero at each node point. The second polynomial has values of zero at each node, slopes of zero at each end point, and a slope of unity at the center node point. These sets of functions are described over the preselected intervals as follows (Price and others, 1968; Doherty, written comm., 1972).

$$w_{2i}(x) = \begin{cases} (-2x + (1+2i)h)(x-(i-1)h)^2/h^3 & ; \ (i-1)h \leq x \leq ih \\ (2x + (1-2i)h)(x-(i+1)h)^2/h^3 & ; \ ih \leq x \leq (i+1)h \\ 0 & \text{otherwise} \end{cases} \tag{39}$$

$$w_{2i+1}(x) = \begin{cases} (x-ih)(x-(i-1)h)^2/h^2 & ; \ (i-1)h \leq x \leq ih \\ (x-ih)(x-(i+1)h)^2/h^2 & ; \ ih \leq x \leq (i+1)h \\ 0 & \text{otherwise} \end{cases}$$

For a one-dimensional problem each basis function is overlain with five adjacent basis functions plus itself. After finite differencing with respect to time there develops sets of linear equations with six unknowns in each equation. For one- and multi-dimensional problems a price is paid in computational efficiency for the advantage of differentiability at node points and fourth-order accuracy.

Inspection of figures 2 and 3 and of equation 32 shows that the solution at a particular node involves the sum of basis functions times the time-dependent coefficient c at that node. This means that the solution at that particular point is equal to the value of the time-dependent coefficient. The Galerkin finite-element method does provide, through equation 32, solutions at any point. Finite-difference methods, however, provide solutions only at nodes, and solutions elsewhere must be obtained by interpolations.

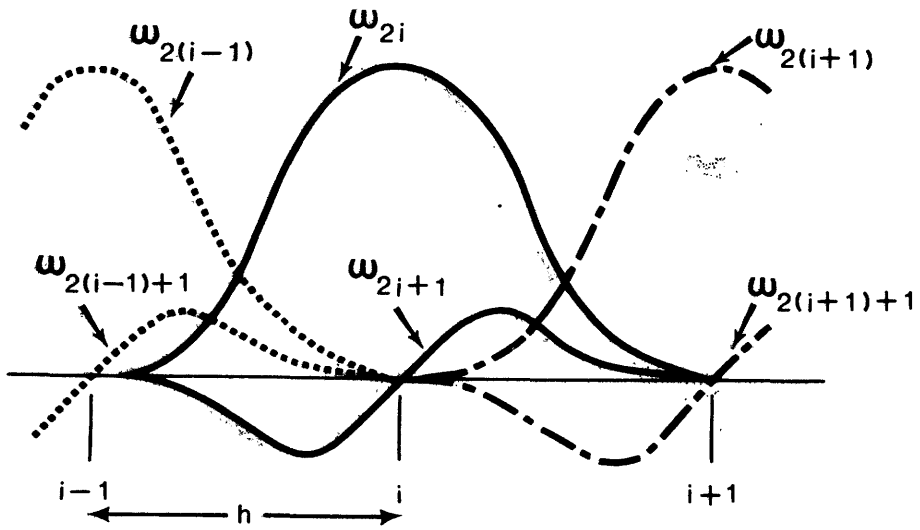


Figure 3.--*Plot of cubic basis functions with grid spacing h.*

Figures 2 and 3 present basis functions for the one-dimensional case. When more than one dimension is required a product of basis functions results. The basis function $v_i(x,y)$ for a rectangular domain in two dimensions can be written as a product of the functions $w_i(x)$ and $w_j(y)$. The function $v_k(x,y)$ can likewise be written $w_k(x)\, w_l(y)$. The Galerkin formulation for the solution of an equation in two dimensions would then be written

$$\iint L\left[\sum_{i=1}^{n}\sum_{j=1}^{m} c_{ij}(t)w_i(x)w_j(y)\right] w_k(x)w_\ell(y)\, dxdy = 0 \quad \text{for } k = 1, 2, \ldots, n \quad \ell = 1, 2, \ldots, m \tag{40}$$

This produces n x m equations with n x m unknowns; however no new mathematical procedures are required for solution. For linear basis functions, nine unknowns are in each equation or row of the matrix, and for the cubic functions, 36 unknowns appear.

Integral evaluation

The solution of equation 35 requires that numerous integrals be evaluated. These integrals may be composed of simple polynomials and in many cases can be evaluated analytically. However, the method is not limited to the use of simple polynomials, such as the linear functions, but can use more complicated functions comprised of cubic and quantic polynomials. Multidimensional equations that result in products of several basis functions should also be considered. Such integrations are certainly more tedious and some cases, more difficult. In this case, it is necessary to resort to numerical integration of the resulting integrals. When chapeau basis functions were used for the one-dimensional problems, integration was done explicitly. Gaussian quadrature was used for one-dimensional problems with cubic basis functions and for all two-dimensional problems. Gaussian quadrature gives exact integrations for polynomials of degree 2n-1 when at least n Gauss points are used; however, satisfactory results can be obtained using less Gauss points.

Gaussian quadrature formulas can be used to integrate functions in the following manner: To integrate

$$Y = \int_a^b f(x)\, dx$$

let

$$t = \frac{2x-(a+b)}{b-a} \tag{41}$$

where

$$x = \frac{b-a}{2} \cdot t + \frac{b+a}{2}$$

then after suitable algebraic manipulation

$$Y_n = (b-a) \sum_{k=1}^{n} \left\{ \frac{A_k^n}{2} \cdot f \left[(b-a) \frac{t_k^n}{2} + \frac{b+a}{2} \right] \right\} \tag{42}$$

where coefficents A_k^n and nodes t_k^n are given in detail by Krylov (1962). For n equals 3 a polynomial of degree 5 can be integrated exactly. For an integration interval of 0 to 1, the Gauss points are located at 0.113, 0.500, and 0.887.

For two-dimensional problems, integration is performed over an area. Procedures for integrating multiple integrals are discussed by Zienkiewiez (1971, p. 148). Integral products of polynomials of degree (2n-1) and (2m-1) require n x m Gauss points for exact integration over the required region. Gauss point locations for n = 3 and m = 3 over a (0,1) X (0,1) grid would have nine locations with respective x and y coordinates of 0.113, 0.5, and 0.887. Position-dependent variables within the differential equation may be evaluated at these Gauss points during the integration procedure. In most cases these variables are assumed constant within the element and evaluated at its center.

Two-dimensional problems with cubic functions result in a sixth-degree polynomial when no space derivatives appear. A three-point quadrature formula is usually accurate enough for this term and all other terms within the equation with space derivatives are integrated exactly. This formula also results in nine points for a two-dimensional element, which is convenient when position dependent variables are evaluated at the Gauss points.

Equation solution methods

It is necessary to select a method to solve the set of linear differential equations illustrated by equation 37. This involves two distinct steps. The first is to approximate the time derivative. This is usually done using finite-difference techniques. The second is to solve the set of algebraic equations resulting from the particular type of differencing selected. These two steps will be discussed separately.

Time derivative approximations

Rewrite the matrix equation as

$$[\alpha] \frac{\overline{dc_i}}{dt} + [\beta] \bar{c}_i = [\lambda] \tag{43}$$

and, as illustrated by equation (13), finite-difference the time derivative in the following manner:

$$[\alpha](\bar{c}_i^{n+1} - \bar{c}_i^{n}) + [\beta]\Delta t \bar{c}_i^{n+\theta} = [\lambda]\Delta t$$

where

$$\bar{c}_n^{n+\Theta} = \Theta\, \bar{c}_i^{n+1} + (1-\Theta)\bar{c}_i^{n} \tag{44}$$

The value given to Θ depends upon the technique used to increment the time value in the equation. When Θ is equal to zero and explicit equation results, and when Θ is equal to one-half an equation centered in time results (known as the Crank-Nicholson method). Finally when Θ is equal to one, a fully implicit (backwards in time) solution results. The most accurate method of time differencing is the Crank-Nicholson approach when theta is equal to one-half. The more stable method of finite differencing is when theta is equal to one and the method is fully implicit. In this analysis theta was chosen equal to one-half.

An alternative way to write the set of algebraic equations resulting from finite differencing with respect to time would be the use of the "residual" in time method (not to be confused with the use of the residual for the weighted-residual methods). Here the difference (residual) in coefficients between time levels at the new and old time level is calculated. This residual in time is defined as

$$\delta\bar{c}_i = \bar{c}_i^{n+1} - \bar{c}_i^{n} \tag{45}$$

By use of this equation $\bar{c}^{n+1}$ is removed from the set of equations and $\delta\bar{c}_i$ is solved for. This technique allows the user more accuracy if the difference between the coefficient values at the initial and later time values are small. This technique was not necessary for the problems examined and therefore was not used.

A set of algebraic linear equations has now been generated that must be solved for the time dependent coefficients.

Matrix solution techniques

Large systems of linear algebraic equations are normally produced when finite-difference and finite-element methods are used to approximate linear differential equations. Two general methods are normally used to solve these large systems of equation: (1) direct methods that use a specific number of computational steps and (2) iterative methods that converge to the answer as the number of computational steps increases. Efficiencies and accuracies of both direct and iterative-solution techniques are usually improved through scaling. The system of linear equations resulting from the two-dimensional finite-element method using cubic basis functions produced a system of equations that required scaling. The associated matrix that described this system was scaled by first dividing each row element by the square root of the diagonal element in its row. Then each column element was divided by the square root of the diagonal element whose row number corresponded to the

column number. This resulted in a matrix diagonal of all ones. The right-hand target vector was divided by the square root of the corresponding diagonal element. After computation the computed value was then rescaled in the same manner as the right-hand target vector yielding the answer. For steady-state conditions, scaling of the associated matrix must only be done once, but the right-hand side vector changed with each time increment and was rescaled each time.

Iteration techniques store only those entries of the matrix with values. Remson and others, 1971, Smith, 1965, and Carnahan, 1969, give in detail iteration methods that solve solutions of systems of linear equations. A study of iteration methods brings out some interesting facets. One is that the conditions sufficient and sometimes necessary for convergence of iteration techniques are not always present for matrices developed through Galerkin finite-element methods. This is not necessarily the case for the simpler one-dimensional equation, but for the more complicated two-dimensional situation the matrix may be quite ill-conditioned.

The one-dimensional problems using cubic basis functions could be solved using successive over relaxation (SOR) as was the two-dimensional equations using linear basis functions. However the matrix generated by the use of cubic basis functions for two dimensions was so poorly conditioned that the traditional iterative methods did not suffice. The author was fortunate to obtain the results of a then unpublished Ph. D. thesis in numerical analysis from the University of Illinois Mathematics Department (T. A. Manteuffel, written commun., 1975) that was able to efficiently solve these sets of equations. The report has since been published (Manteuffel, 1975) and the interested reader is referred to the original reference for a complete discussion.

Direct methods, in general, are less susceptible to convergence problems caused by ill-defined matrices than are iteration methods. The problems with direct methods are that they may be long and tedious and sometimes require great storage arrays to produce adequate solutions. Typical examples of these methods would be matrix inversion and Gaussian elimination.

There are instances, however, when sparse matrices lend themselves to certain techniques of solving equations. For example, when the matrix is composed of bands of elements leading down and adjacent to the diagonal it is sometimes possible to use specific linear-equation solution techniques that only use storage of, and computation on, these bands of equations. Gaussian elimination is then performed on a reconstructed matrix describing these equations. The Thomas algorithm for a tridiagonal matrix as obtained for a one-dimensional problem is an example of this solution technique.

The two-dimensional system produced by the cubic basis functions was solved for small sets of equations using an IBM band solve routine DGELB. Manipulation of the associated matrix to conform to the banded structure while preserving low storage was somewhat difficult. The associated matrix and right-hand side vector were scaled by dividing each row by its largest absolute value. Columnwise scaling was unnecessary due to pivoting during the Gaussian elimination solution procedure. Large systems of equations produced wide band-widths and excessive storage requirements. Therefore this technique was used for small or moderate-sized programs.

APPLICATION OF THE GALERKIN FINITE-ELEMENT METHOD TO THE SOLUTION OF MASS-TRANSPORT EQUATIONS

In this section, solution procedures for the mass-transport equation will be constructed. Analytical solutions for one of the simpler cases will be compared with the solutions obtained from the Galerkin finite-element technique. For more complex multidimensional problems the finite-element method will be compared with finite-difference solutions.

Solution of the mass-transport equation involving both hyperbolic and parabolic problems will now be discussed in detail. Included will be solution techniques for both one- and two-dimensional mass-transport equations with and without chemical reactions.

One-dimensional solutions

An example of a finite-element solution to a one-dimensional mass-transport equation is given by solving the one-dimensional diffusion convection equation without chemical reactions.

$$L[c] = \frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0 \tag{46}$$

The x dimension is first divided into n-1 finite elements and n nodes. The basis functions are defined over the domain of interest. The residual is formed by substituting this approximation into the differential equation for the dependent variable c. Galerkin's technique is applied to the residual by multiplying it by the weighting functions and integrating it over the interval of interest. The following sets of n integral equations with unknowns c(t) and c'(t) results.

$$\int_0^L \sum_{i=1}^{n} c_i'(t)w_i(x)w_k(x)dx + \int_0^L v\sum_{i=1}^{n} c_i(t)w_i'(x)w_k(x)dx$$

$$-\int_0^L D\sum_{i=1}^{n} c_i(t)w_i''(x)w_k(x)dx = 0 \text{ for } k = 1,2, \ldots, n \tag{47}$$

where superscript prime (') indicates differentiation and w_i and w_k denote the approximating and weighting functions, respectively.

For every weighting function or value of k there exists a linear-differential equation. Equation 47 thus represents a set of n linear-differential equations.

The equations that best define the conditions at the boundaries are the flux conditions given by Brenner (1962) as

$$D\frac{\partial c}{\partial x} = -v(c - c_o), \qquad \text{for } x = 0,\ t \geq 0,$$

$$\frac{\partial c}{\partial x} = 0, \qquad \text{for } x = L,\ t \geq 0. \tag{48}$$

When it is important to specify exact boundary conditions, basis functions and their respective time-dependent coefficients are chosen to take on the required characteristics at the boundaries. For equation 48, boundary conditions are those given by Brenner (1962), and basis functions that provide proper solutions at the boundaries must be adaptable to these boundary equations. Substitution of the approximation for the dependent variable into these boundary equations results in the following:

$$D\sum_{i=1}^{n} c_i(t)w_i'(o) = v\sum_{i=1}^{n}\left[c_i(t)w_i(o) - c_o\right] \quad \text{for } x = 0 \tag{48a}$$

$$\sum_{i=1}^{n} c_i(t)w_i'(L) = 0 \qquad \text{for } x = L \tag{48b}$$

Equation 48b requires that the basis functions at x = L have a slope equal to zero. Cubic functions automatically have this property; however, linear functions do not. The n-1 and n linear basis functions are therefore modified to give them this property. They are redefined in the following manner:

$$w_{n-1}(x) = \begin{cases} (x-(n-2)h)/h & ;\ (n-2)h \leq x \leq (n-1)h \\ (nh-x)^2/h^2 & ;\ (n-1)h \leq x \leq nh = 1 \end{cases}$$

$$w_n(x) = ((x-nh)^2-h^2)/h^2 \qquad ;\ (n-1)h \leq x \leq mh = 1 \tag{49}$$

The defining equation 46 contains second-order derivatives. Unless the basis functions can be differentiated twice, a trivial solution results. This problem is rectified by integrating all second derivatives by parts.

Such integration performed on the last term in equation 47 results in the following

$$-D\int_{o}^{L}\sum_{i=1}^{n} c_i(t)w_i''(x)w_k(x)dx = -\left[D\sum_{i=1}^{n} c_i(t)w_i'(x)w_k(x)\right]_{o}^{L}$$

$$-D\int_{o}^{L}\sum_{i=1}^{n} c_i(t)w_i'(x)w_k'(x)dx \quad \text{for } k = 1, 2, \ldots, n \tag{50}$$

Combining 47, 48, and 50 the following equation is obtained.

$$\int_{o}^{L}\sum_{i=1}^{n} c_i'(t)w_i(x)w_k(x)dx + \int_{o}^{L} v\sum_{i=1}^{n} c_i(t)w_i'(x)w_k(x)dx$$

$$+ v\left[c_1(t)-c_o\right]w_k(o) + \int_{o}^{L} D\sum_{i=1}^{n} c_i(t)w_i'(x)w_k'(x)dx = 0 \text{ for } k = 1, 2, \ldots, n \tag{51}$$

The next step is to substitute the basis functions into equation 51 and integrate. This results in a set of linear differential equations in time.

The coefficient matrix that results from the analytical integration of the simple one-dimensional example using linear basis functions is given below.

$$h \cdot \begin{bmatrix} 1/3 & 1/6 & & & & \\ 1/6 & 1/3 & 1/6 & & & \\ & 1/6 & 1/3 & 1/6 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1/6 & 8/15 & 2/15 \\ & & & & 2/15 & 8/15 \end{bmatrix} \cdot \begin{bmatrix} dc_1/dt \\ dc_2/dt \\ dc_3/dt \\ \vdots \\ dc_{n-1}/dt \\ dc_n/dt \end{bmatrix} +$$

$$\frac{D}{h} \cdot \begin{bmatrix} A1 & -A2 & & & & & \\ -A1 & 2 & -A2 & & & & \\ & -A1 & 2 & -A2 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & -A1 & 7/3 & -A4 \\ & & & & & -A3 & A3 \end{bmatrix} \cdot \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{n-1} \\ c_n \end{bmatrix} = \begin{bmatrix} Vc_o \\ o \\ o \\ o \\ o \\ o \\ o \\ o \end{bmatrix} \quad (52)$$

where $A1 = 1+\alpha$

$A2 = 1-\alpha$

$A3 = 4/3+\alpha$

$A4 = 4/3-\alpha$

and $\alpha = \frac{Vh}{2D}$

This set of equations is solved by finite-differencing the time derivative using the Crank-Nicholson method. The differential equation describing one-dimensional flow through porous medium is difficult to solve accurately numerically for low values of the dispersion coefficient because of oscillation or numerical dispersion. Figures 4 and 5 present numerical and analytical solutions, respectively, of equation 46 for dispersion coefficients of 0.001 and 0.0001. This equation was solved using the Galerkin finite-element method with both linear and cubic basis functions for time steps of 0.002 and a space increment of 0.1. The column length and fluid velocity were both 1.0. A space and time-centered finite-difference technique was used to solve this equation. Severe oscillations of the finite-difference solution results for both values of dispersion coefficients. These results demonstrate that sharp fronts, that is, those with low dispersion coefficients, are difficult to model with standard, finite-difference methods. Note, however, that for figure 4, Galerkin finite-element techniques using linear and cubic functions closely match the analytical solution. For very low values of the dispersion coefficient (fig. 5) the chapeau functions produce oscillation.

Two-dimensional solutions

The advantage of finite-element techniques becomes apparent with the solution of the two-dimensional, diffusion-convection equation where small dispersion coefficients predominate. There is basically no difference in the formation of the residual that must be minimized under the integral than was done with the one-dimensional transport equation. The general transport equation to be solved is equation 7.

As with the one-dimensional equation, second-order differentials appear and must be reduced to first order. As shown previously, these terms appear in the description of the dispersion process and are

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial x}\left(D_{xy}\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c}{\partial x}\right) \tag{53a}$$

These terms are differentiated and the residual is formed to obtain

$$\int_{y_o}^{y_L}\int_{x_o}^{x_L}\left[D_{xx}\frac{\partial^2 c}{\partial x^2}+\frac{\partial D_{xx}}{\partial x}\frac{\partial c}{\partial x}+D_{yy}\frac{\partial^2 c}{\partial y^2}+\frac{\partial D_{yy}}{\partial y}\frac{\partial c}{\partial y}+D_{xy}\frac{\partial^2 c}{\partial x\partial y}\right.$$

$$\left.+\frac{\partial D_{xy}}{\partial x}\frac{\partial c}{\partial y}+D_{yx}\frac{\partial^2 c}{\partial y\partial x}+\frac{\partial D_{yx}}{\partial y}\frac{\partial c}{\partial x}\right]w_k(x)w_\ell(y)\,dx\,dy \tag{53b}$$

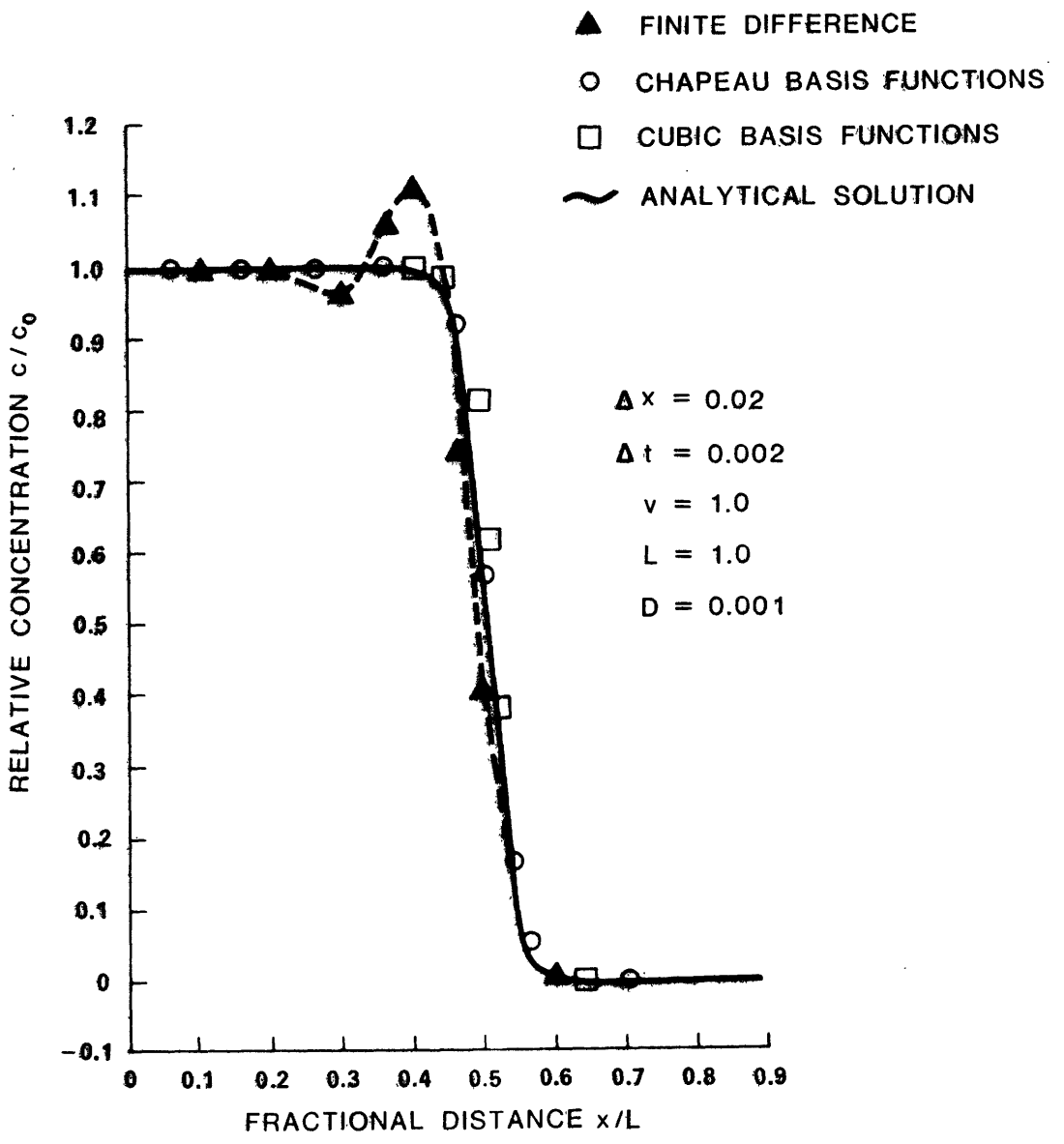


Figure 4.--*Comparison of finite-difference and finite-element solutions to the convective-diffusion equation for a dispersion coefficient of* 0.001 *and a displaced pore volume of* 0.5.

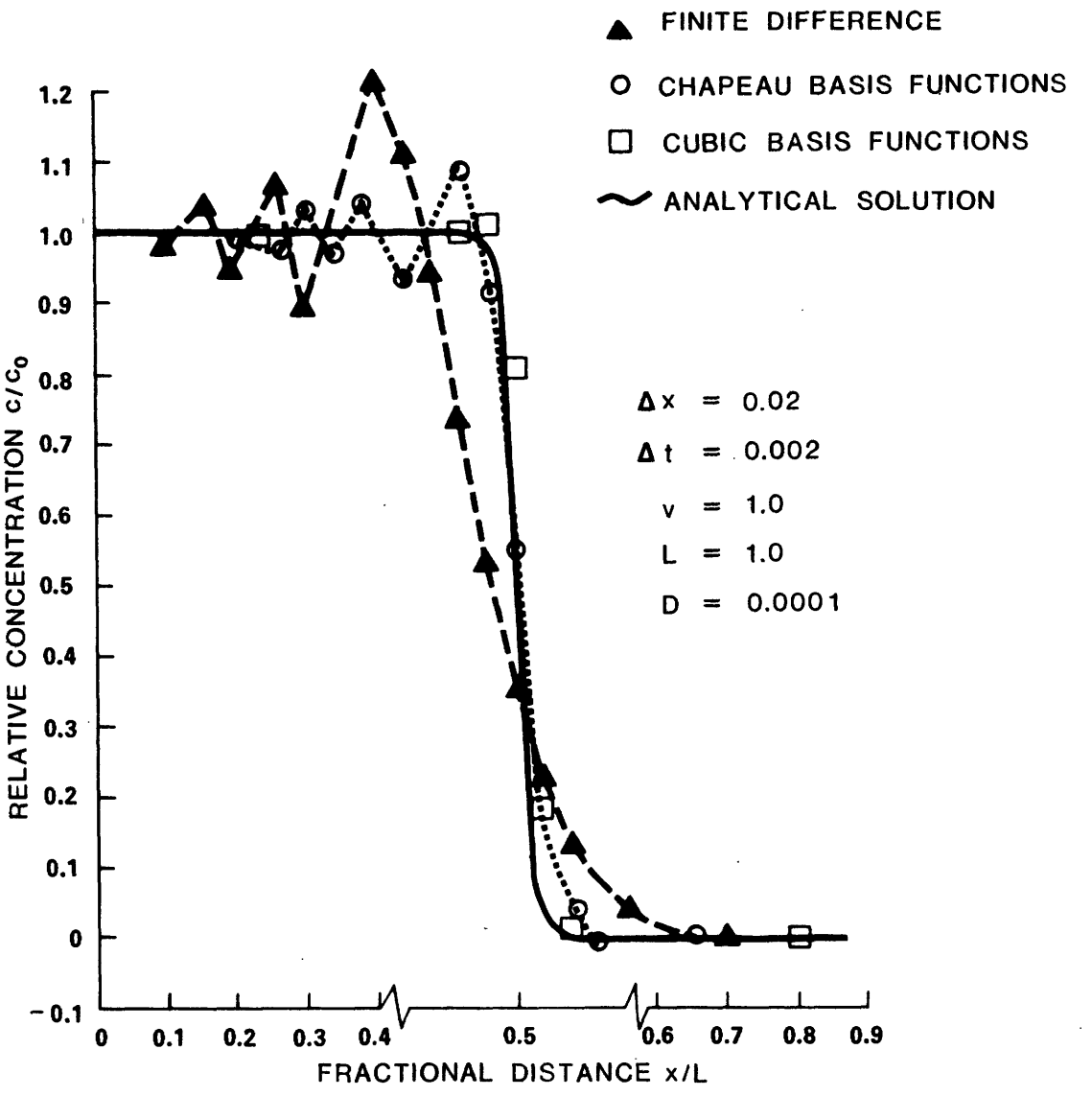


Figure 5.--*Comparison of finite-difference and finite-element solutions to the convective-diffusion equation for a dispersion coefficient of* 0.0001 *and a displaced pore volume of* 0.5.

Reduction to first order is accomplished by integration by parts. Integration of this equation can be done in an elegant manner using vector calculus as illustrated generally (Wylie, 1966, p. 572) and specifically (Pinder and others, 1973) for the flow equation.

Since this integration may produce terms for inclusion into the boundary equations, a detailed integration by parts will be performed for the first of the integral terms:

$$u = D_{xx} w_{k_\ell} \ (x,y) \text{ where } w_{k_\ell}\ (x,y) = w_k(x) w_\ell\ (y)$$

$$dv = \frac{\partial^2 c}{\partial x^2}\, dx$$

therefore

$$du = D_{xx} \frac{\partial w_{k\ell}\ (x,y)}{\partial x} + w_{k\ell}\ (x,y) \frac{\partial D_{xx}}{\partial x}$$

$$v = \int \frac{\partial^2 c}{\partial x}\, dx = \frac{\partial c}{\partial x}$$

then the first term of equation 53 becomes

$$\int_{y_o}^{Y_L} \left[D_{xx} w_{k\ell} \frac{\partial c}{\partial x} \right]_{x_o}^{x_L} dy - \int_{y_o}^{y_L} \int_{x_o}^{x_L} \left[D_{xx} \frac{\partial w_{k\ell}}{\partial x} \frac{\partial c}{\partial x} + w_{k\ell} \frac{\partial D_{xx}}{\partial x} \frac{\partial c}{\partial x} \right] dxdy$$

Performing this integration on all of the second-ordered derivatives results in the following equation:

$$\int_{y_o}^{y_L} \left[D_{xx} w_{k\ell} \frac{\partial c}{\partial x} + D_{xy} w_{k\ell} \frac{\partial c}{\partial y} \right]_{x_o}^{x_L} dy + \int_{x_o}^{x_L} \left[D_{yy} w_{k\ell} \frac{\partial c}{\partial y} + D_{yx} w_{k\ell} \frac{\partial c}{\partial x} \right]_{y_o}^{y_L} dx$$

$$- \int_{y_o}^{y_L} \int_{x_o}^{x_L} \left[D_{xx} \frac{\partial c}{\partial x} \frac{\partial w_{k\ell}}{\partial x} + D_{yy} \frac{\partial c}{\partial y} \frac{\partial w_{k\ell}}{\partial y} + D_{xy} \frac{\partial c}{\partial x} \frac{\partial w_{k\ell}}{\partial y} + D_{yx} \frac{\partial c}{\partial x} \frac{\partial w_{k\ell}}{\partial x} \right] dxdy \qquad (54)$$

The series approximation for the dependent variable (concentration) for the two-dimensional, mass-tranport equation is given as

$$c_{n,m}(t,x,y) = \sum_{i=1}^{n} \sum_{j=1}^{m} c_{ij}(t) w_i(x) w_j(y) \tag{55}$$

As mentioned previously, integration of two-dimensional problems is carried out over the element area by mathematical operations at positions located at Gauss points within the element. When parameters were known to change rapidly with position, selected finite elements (in the area of rapid change) were subdivided into nine subelements, the centers of each closely corresponding to the Gauss points. Position-dependent variables were evaluated at each of these points. This procedure was used only for elements using cubic basis function and only for elements surrounding nodes that described wells. A complete subdivision of all finite elements in this manner was successfully accomplished but deemed impractical for large-scale problems.

The two-dimensional form of the mass-transport equation, where the chemical reaction term is assumed to be equilibrium-controlled ion exchange with a first-order irreversible chemical reaction, is now written as

$$\sum_{i=1}^{n} \sum_{j=1}^{m} \int_{o}^{y_L} \int_{o}^{x_L} \Bigg\{ c'_{ij}(t) w_i(x) w_j(y) w_k(x) w_\ell(y) + c_{ij}(t) \Bigg[v_x w'_i(x) w_j(y) w_k(x) w_\ell(y)$$

$$+ v_y w_i(x) w'_j(y) w_k(x) w_\ell(y) + D_{xx} w'_i(x) w_j(y) w'_k(x) w_\ell(y)$$

$$+ D_{yy} w_i(x) w'_j(y) w_k(x) w'_\ell(y) + D_{xy} w'_i(x) w_j(y) w_k(x) w'_\ell(y)$$

$$+ D_{yx} w_i(x) w'_j(y) w'_k(x) w_\ell(y) - \frac{Q}{\epsilon} w_i(x) w_j(y) w_k(x) w_\ell(y)$$

$$+ k w_i(x) w_j(y) w_k(x) w_\ell(y) \Bigg] \Bigg\} dx dy$$

$$+ \sum_{i=1}^{n} \sum_{j=1}^{m} c_{ij}(t) \left\{ \int_{o}^{y_L} \left[(D_{xx} W'_i(x) w_j(y) + D_{xy} w_i(x) w'_j(y) w_k(x) w_\ell(y) \right]_{o}^{x_L} dy \right.$$

$$\left. + \int_{o}^{x_L} \left[(D_{yy} w_i(x) w'_j(y) + D_{yx} w'_i(x) w_j(y) w_k(x) w_\ell(y) \right]_{o}^{y_L} dx \right\}$$

$$+ \int_{o}^{y_L} \int_{o}^{x_L} \frac{c_w Q}{\epsilon} w_k(x) w_\ell(y) \, dx dy = 0 \qquad \begin{array}{l} \text{for } k = 1, 2, \ldots, n \\ \quad\; \ell = 1, 2, \ldots, m \end{array} \tag{56}$$

Integration of equation 56 produces a set of n x m linear differential equations. The integrals are evaluated using Gaussian numerical-quadrature methods as previously discussed. Each algebraic equation will have as many as 9 unknowns for chapeau basis functions and 36 unknowns for cubic basis functions depending on its type and closeness to the boundary. As was the case with the one-dimensional problems, the basis functions require that the coefficient value $c_{ij}(t)$ is also the value of the variable $c_{n,m}(x,y,t)$ for linear basis functions and where the product of the basis functions equal one for the cubic functions.

The matrix differential equation that expresses equation 56 after integration can be written

$$[\alpha] \frac{\overline{dc_{ij}}}{dt} + [\beta] \overline{c_{ij}} = [\lambda]$$

This equation is then finite differenced with respect to time in the Crank-Nicholson manner and the previously mentioned techniques used to solve the resulting matrix.

The two-dimensional, finite-element solution was compared to an analytical solution as was the one-dimensional case. Unidirectional flow in the x or y direction was imposed on the two-dimensional equation without sinks, sources, or chemical reactions. The breakthrough curves, for a problem with boundary conditions similar to those used for the one-dimensional equation, were identical to those obtained for the one-dimensional analytical and numerical solution.

The finite-element programs were also compared with a previously developed finite-difference model. The finite-difference program has been used previously within the U.S. Geological Survey and checked extensively with analytical solutions to known problems, with satisfactory results. A hypothetical waste-contamination problem was used to demonstrate the compatibility of all three models. Two finite-element models, using chapeau and cubic basis functions, respectively, were used in the simulation study.

The physical system is schematically represented as figure 6. An injection well introduced a conservative solute into an areal-flow field directed southward and a pumping well intercepting a portion of the injected fluid during its travel. Figures 7 and 8 give solute concentrations at areal nodal points directly beneath the injection well and at the intercepting well as a function of time. The notation (refined) for one of the simulations using hermite cubic basis indicates more detailed definition of solution parameters at nine gauss points within the finite element. Exact comparisons should not be expected; however, the closeness of values for these widely different types of numerical analysis is apparent.

APPLICATION OF THE GALERKIN FINITE-ELEMENT TECHNIQUE TO A FIELD PROBLEM

The Galerkin finite-element method has been shown in the previous chapters to adequately simulate known analytical solutions to mass-transport equations.

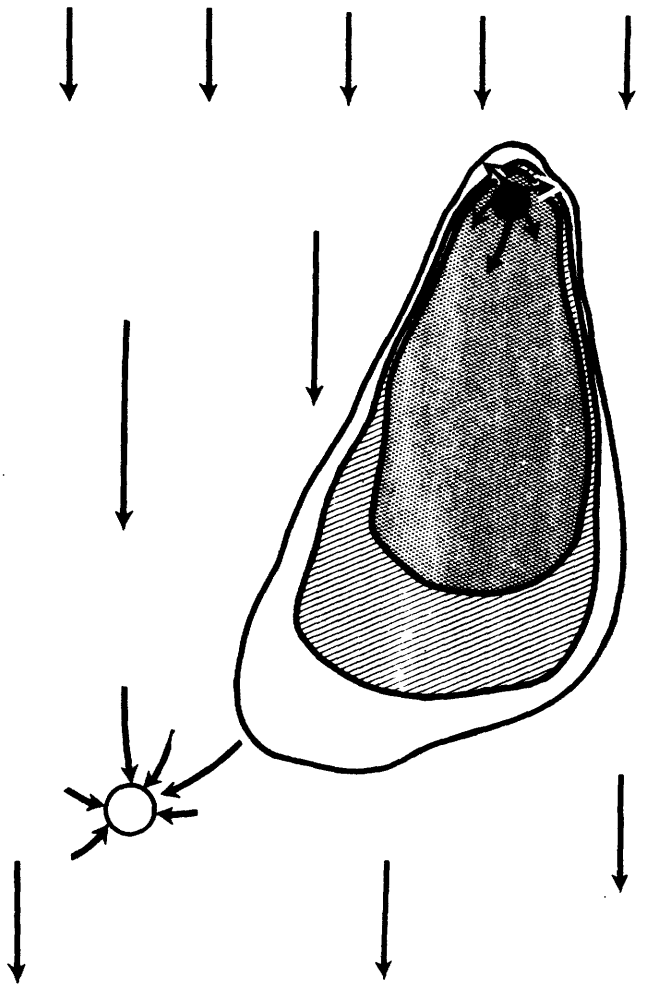


Figure 6.--*A schematic representation of a two-dimensional solute transport problem*

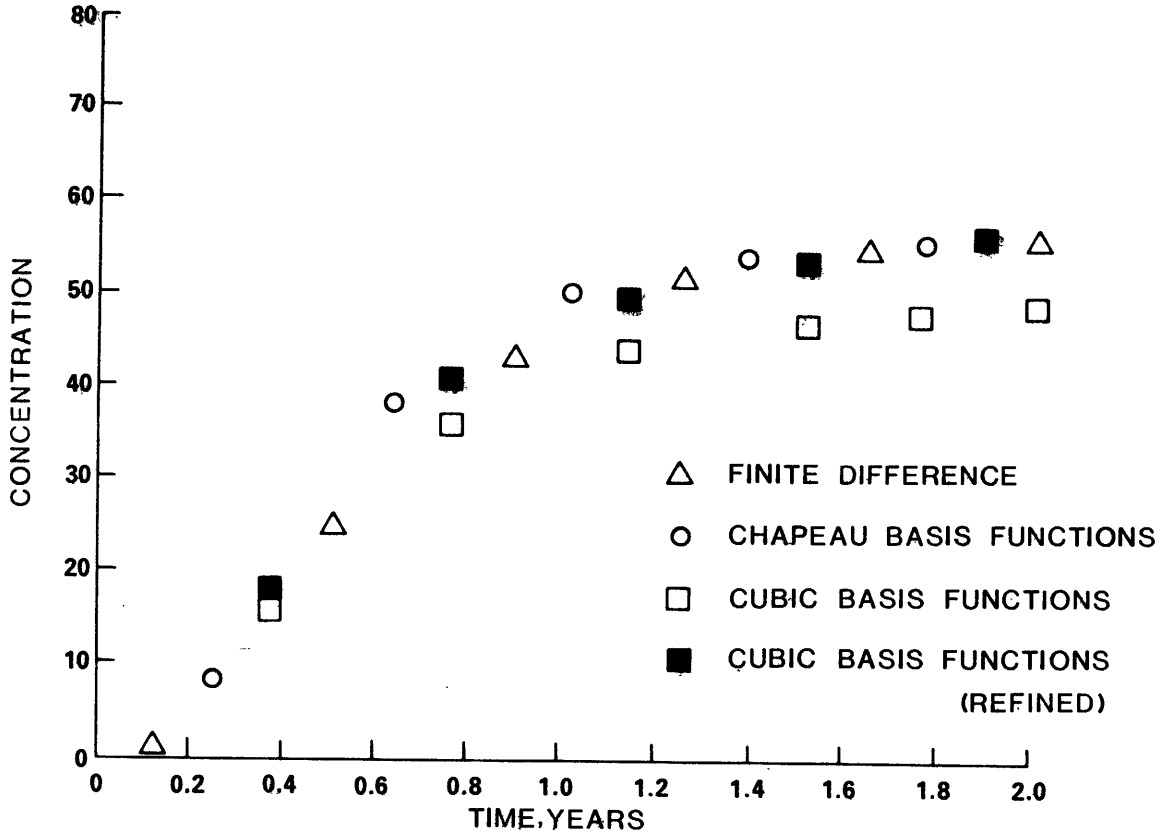


Figure 7.--*A comparison of numerical techniques for a simulated two-dimensional transport problem for a point directly beneath the well.*

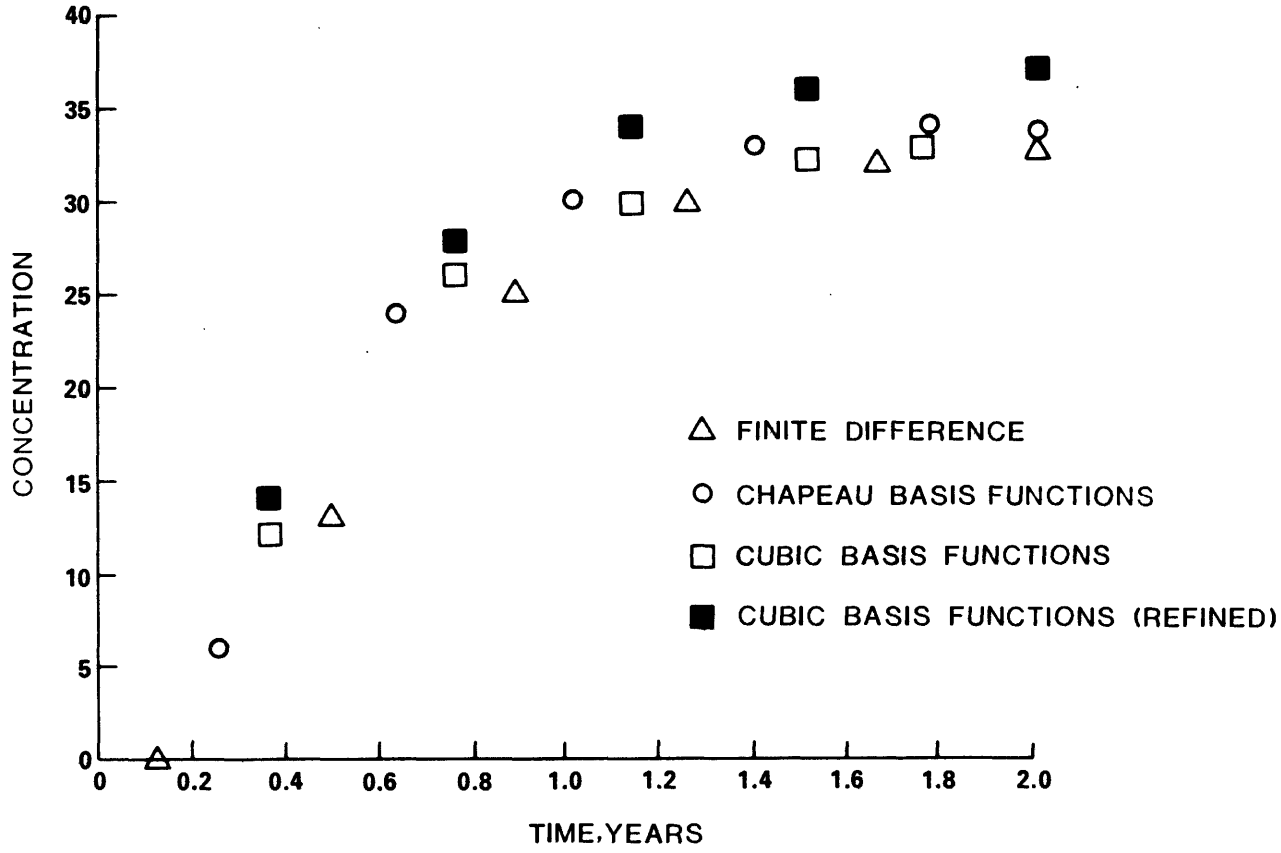


Figure 8.--*A comparison of numerical techniques for a simulated two-dimensional transport problem for the intercepting well.*

In this section the method will be applied to a known ground-water contamination problem. The area is the Snake River plain aquifer at the Idaho National Engineering Laboratory (INEL), which was formally called the National Reactor Testing Station in Idaho. Robertson (1974) modeled the movement of waste through this aquifer using finite-difference techniques for the flow model and the method of characteristics for the solute-transport model.

The reason that this particular area was chosen is that excellent field data are available and the waste reacts chemically during its movement through the aquifer.

Problem description

Robertson, Schoen, and Barraclough (1974) gave a detailed geographic, geologic, and hydrologic description of the Snake River aquifer underlying the INEL (Idaho National Engineering Laboratory). The reader interested in such details is referred to reports by these authors. This manuscript deals with one small part of their work; therefore, only an abbreviated description of the area and the waste-disposal problem will be given here.

The INEL is located on the Snake River Plain in southeastern Idaho. This plain is underlain by the Snake River plain aquifer that is made up of numerous basaltic flows and contains a vast amount of ground water. Ground water is recharged in the higher mountains and flows to the southwest through very hetrogeneous basalt discharging through springs into the Snake River. A pictorial map depicting the generalized ground-water flow pattern and salient surface features is shown in figure 9.

Since 1952 chemical and low-level radioactive wastes are disposed of into the ground-water system. These wastes migrate down the hydraulic gradient and, unless removed from the aquifer by physical or chemical means, will eventually discharge into the Snake River. The majority of the wastes were injected into the aquifer at two sites; the TRA (Test Reactor Area) and the ICPP (Idaho Chemical Processing Plant). Robertson (1974) gave the input rate for waste-water recharge for these two sites and these are shown in table 2. Figure 10 illustrates the regional ground-water table, May through June 1965, the location of the waste-water recharge sites, and the area chosen to be modeled for solute transport.

Sampling of the waste products was accomplished through monitor wells drilled down gradient from the injection points. The background level for chloride was 10-20 mg/L. The monitoring of tritium and strontium was limited by the detection level of the analysis procedure which was 2 pCi/mL for tritium and 0.005 pCi/mL for strontium.

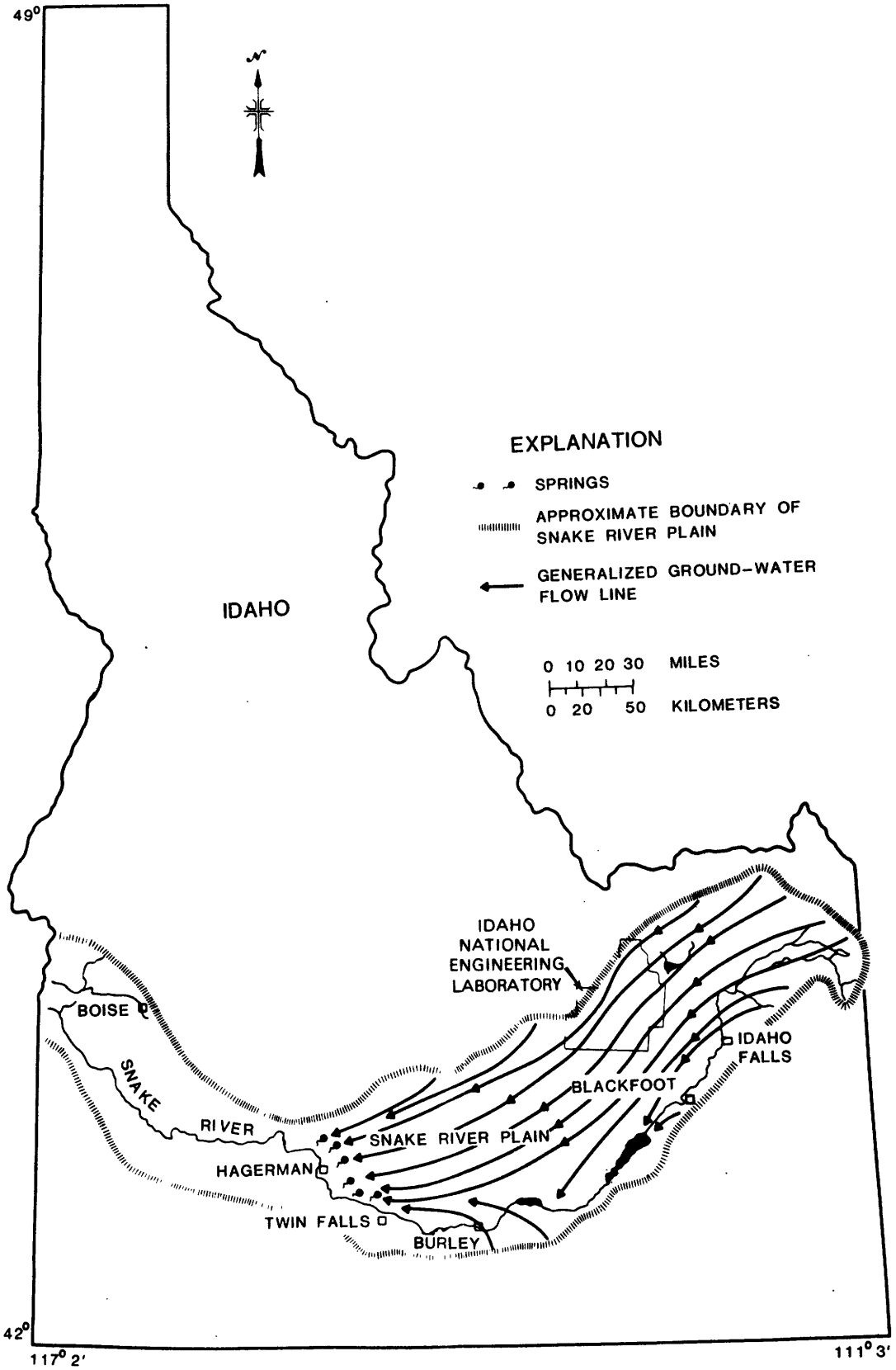


Figure 9.--*Map of Idaho showing the location of the INEL, the Snake River Plain, and inferred ground-water flow lines (from Robertson, 1974).*

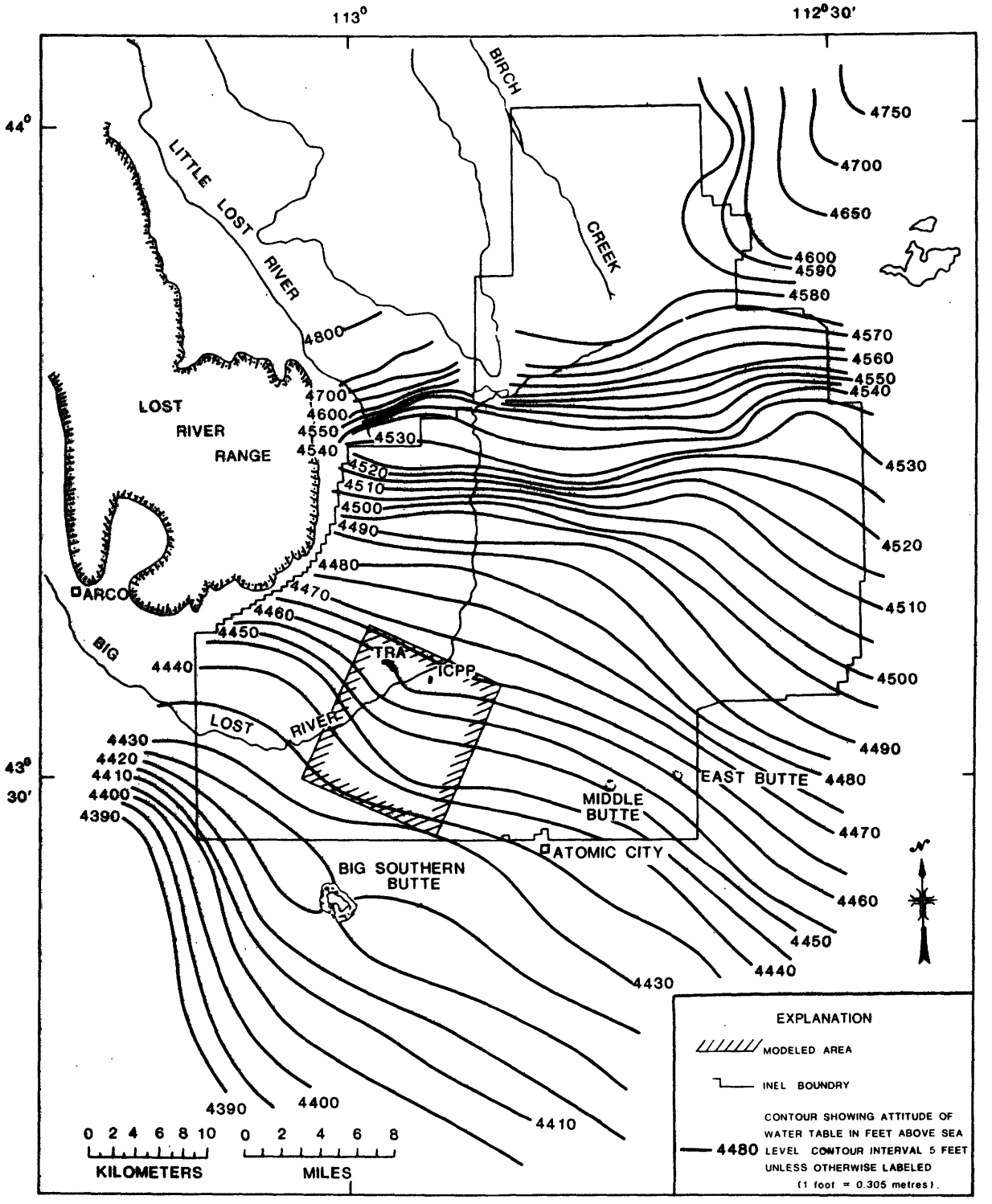


Figure 10.--*The regional ground-water table, May through June 1965, the location of the waste-water recharge sites, and the modeled area at INEL, Idaho, (Robertson, 1974).*

Table 2.--*Input rates and concentrations for waste-water recharge at INEL, Idaho*

[mg/L is milligrams per liter; pCi/mL is pico curies per milliliter; ft^3/s is cubic feet per second; cm^3/s is cubic centimeters per second.]

	TRA	ICPP
Chloride (Cl^-)	35 mg/L	245 mg/L
Tritium (H^3)	300 pCi/mL	800 pCi/mL
Strontium-90 (Sr^{90})	0.0	1.0 pCi/mL
Injection rate	1.9 ft^3/s (0.054 cm^3/s)	1.7 ft^3/s (0.048 cm^3/s)

Movement of these three products through the ground-water system depends on chemical as well as physical factors. The physical factors are the previously discussed effects of convective transport and dispersive transport, the latter being used to approximate nonideal flow conditions. The chemical factors may include rate reactions and ion exchange. The former is characterized in this instance by radioactive decay of the tritium and the strontium. The latter is characterized solely by the strontium where the small chemical concentrations allow the assumption of linear-adsorption isotherms. Since surface-controlled ion exchange (as we would expect here) is usually very fast, equilibrium conditions are assumed and the previously developed equations covering this case apply.

Chloride is a nonreactive waste species that is used to characterize the system in terms of the dispersion coefficient. Matching observed with numerically-derived data allows determination of dispersivity constants and gives some check on the accuracy of the determined velocities that control the convective transport portion of the transport equation. Using this technique a longitudinal characteristic length of 300 feet and a ratio of $\alpha_L/\alpha_r = 1$ was chosen for this test problem.

The chemical parameters necessary to the solution of the transport equation are now discussed. Equation 26 illustrates the first-order rate constant for radioactive decay to be 0.693/half life. The half life of tritium is 12.26 years and for strontium-90 is 28.9 years. The respective rate constants for tritium and strontium are then 0.0565 yr^{-1} and 0.0240 yr^{-1}.

Since a linear adsorption isotherm can be used to characterize the exchange process a distribution coefficient is required. The determination of a dis-distribution coefficient that will apply to field situations is difficult. Robertson (1974) reported that of the strontium injected into the system only 3 percent is present in the aqueous phase. The rest is assumed to be adsorbed on the surface of the aquifer matrix. This information allows calculation of a term related to the distribution coefficient that can be used to calculate the effect of ion exchange. The term $K_d\rho_b/\varepsilon$ in equation 28 can be shown for these conditions to be equal to 0.97/0.03 or 32.33. The retardation factor defined by equation 29 is then 33.33. This information can be translated to mean that the average velocity of the strontium ion is traveling 0.03 times the velocity of the ground water.

Initial conditions for contaminants in the ground-water system assumed that neither tritium nor strontium were present. As mentioned previously, the background level of chloride was assumed to be 10 mg/L.

Simulation of contamination conditions

As illustrated by figure 10, an area of INEL approximately 8 x 8 mi was chosen to be modeled for the transport of waste solutes. This area was then divided into 20 x 20 finite-difference cells. These finite-difference cells were used to calculate the detailed head distribution using the finite-difference approximation to the flow equation. The finite-element net was then overlain on top of the finite-difference cells with the finite-element node falling on the center of the finite-difference cell. The finite-element area then comprised quarter portions of four finite-difference cells. This program allows the use of existing finite-difference solutions to the simpler equations that define the hydraulic head in the aquifer. The length of the sides of the elements and cells was 2,100 ft (640 m). Figure 11 illustrates the finite-difference and finite-element nodes as used for the INEL contamination problem. The boundaries are approximated by a zero concentration gradient. This is accomplished by setting the concentration of the boundary node equal to the adjacent node or a fixed initial concentration, depending on the direction of the velocity.

In detail, the modeled area contained four wells, two discharging (pumping) and two recharging waste water.

All finite-element simulation studies were done using linear basis functions. Computer runs for identical problems using the cubic basis functions took an order of magnitude longer for CPU time. When larger size elements were used to decrease the size of the matrices, the necessary detail for problem solution was lost. The use of cubic basis functions is recommended for situations where uniform conditions exist throughout the medium, thus allowing fewer elements to be used. Further research on means to generate more detail within the larger finite elements which must be used with the cubic basis functions, or more rapid solution techniques for sparce, poorly conditioned matrices, might allow expanded use of this method. Using the input data from table 1, concentration maps were generated for chloride, tritium, and strontium. These generated profiles were compared with field data contoured by Robertson (1974).

Chloride contamination simulation

Figure 12 compares the waste-chloride plumes for 1968-69 based on well-sample data and the finite-element model using the linear basis functions. Comparisons between field and computer simulations are considered good for this type of study. Field generated contours, such as the 15-mg/L isochlor, were in some cases estimates based on one or two sample points. The material balance of the simulation study indicated an 8-percent error for this run of 17.1 years.

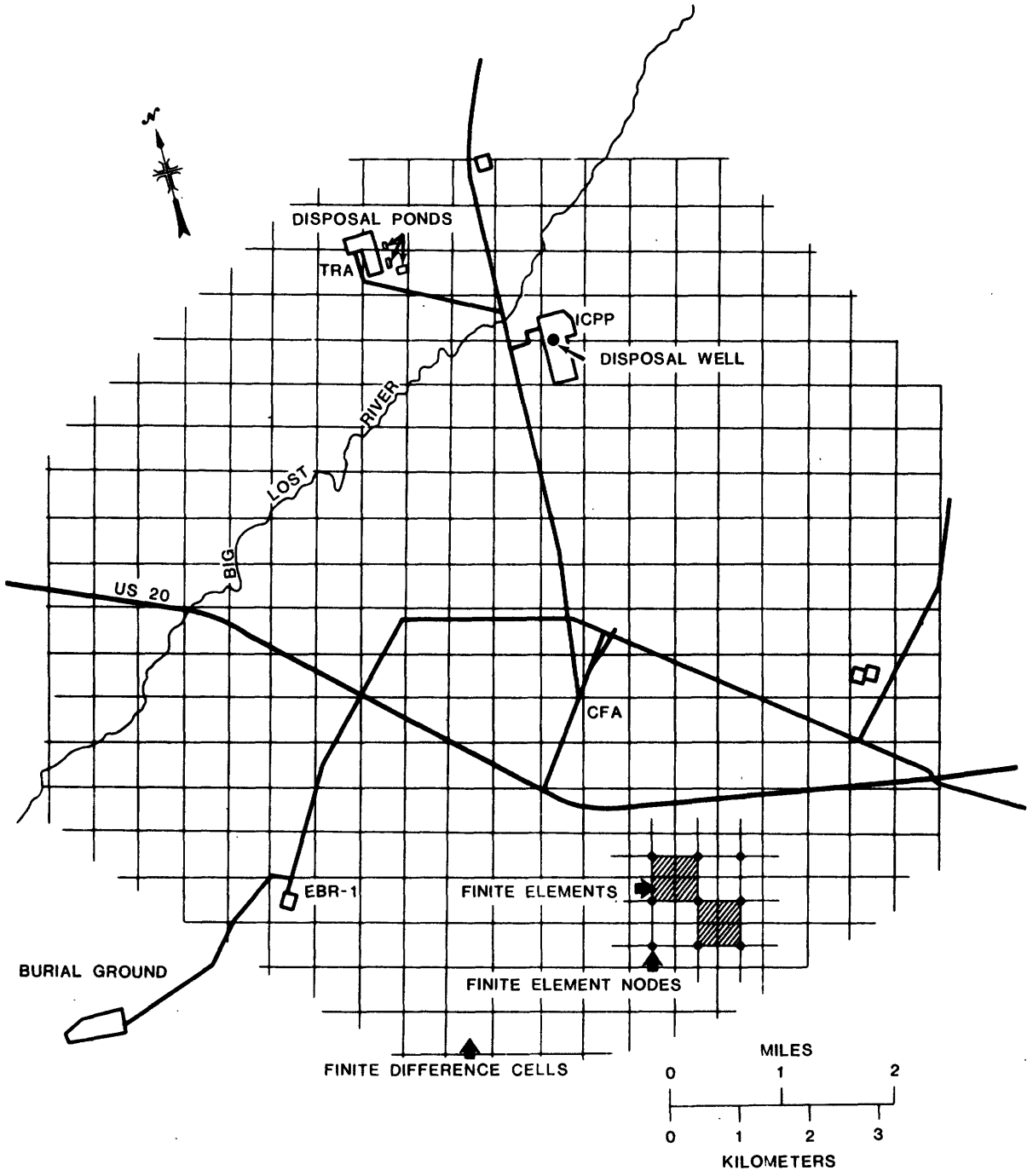


Figure 11.--*Location of finite-difference cells and finite-element nodes for the NRTS contamination problem*

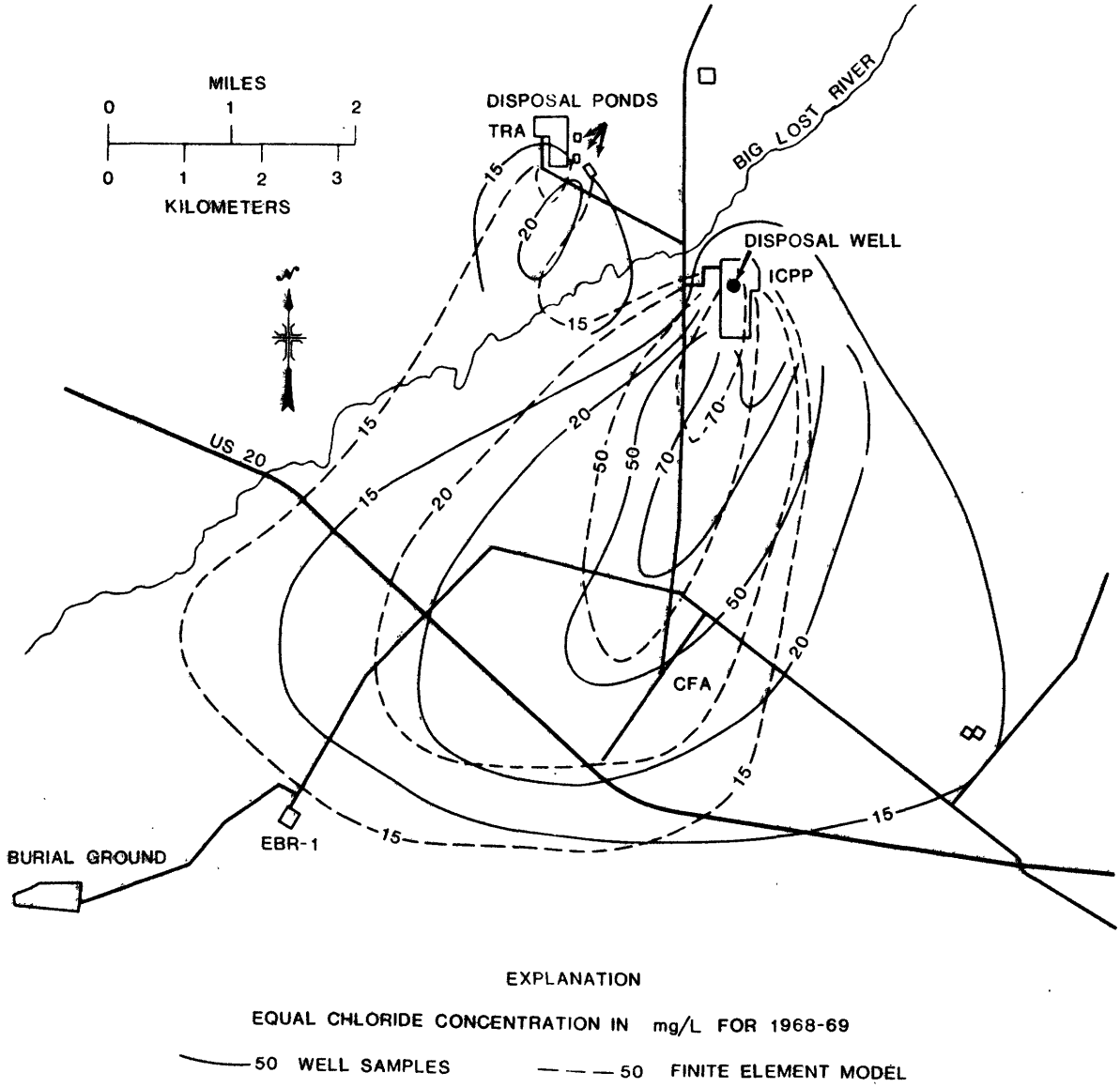


Figure 12.--*Comparison of waste chloride plumes for 1968-69 based on well sample data and computer model.*

Tritium contamination simulation

Figure 13 compares the waste-tritium plumes for 1968-69 based on well-sample data and the finite-element model using the linear basis functions. The introduction of an irreversible chemical-reaction term to account for radioactive decay distinguishes this simulation from the chloride. Except for the introduction of this term and the different initial and boundary conditions, the mass-transport parameters were the same. Excellent correlation between the field data contours and finite-element contours again resulted.

Strontium contamination simulation

Strontium-90 was injected only into the ICPP disposal well at relatively low concentrations. The high degree of ion exchange retards the movement of this radioactive species through the ground-water system. This chemical reaction adds a term to the equation to simulate a retarded movement of the ion. Figure 14 compares numerical-calculated versus field-observed data for the strontium contamination problem. Although it is difficult to make accurate comparisons for this small movement, adequate comparisons of the field and computed data exist.

SUMMARY AND CONCLUSIONS

The use of Galerkin finite-elements to solve the partial-differential equation that describes mass transport was shown to be a feasible approach. The use of linear and cubic basis functions generated solutions to the convective-diffusion equation that were more accurate and less susceptible to oscillation than finite-difference methods. Large-scale two-dimensional problems can be solved with these methods; however, excessive computer time results with the use of cubic basis functions. This is due to the structure of the coefficient matrix that represents the system of differential equations that must be solved. Linear basis functions form strongly diagonal matrices with no more than nine entries per row. Cubic basis functions form matrices with weak diagonals and as many as 36 elements per row. The use of SOR to solve the matrix formed with linear functions was very efficient. A more involved iterative technique was necessary to solve the matrix generated by the cubic functions. A sample problem required a factor of 10 times longer CPU time to solve the problem using cubic functions rather than the linear functions. This time difference can perhaps be lessened by using fewer but larger sized elements for the cubic equations. The decrease in program sensitivity to parameter values such as areal changes in transmissivity and well locations makes this adjustment presently unattractive.

The model's practical use was demonstrated by solving field-contamination problems. The concentration profiles of chloride, tritium, and strontium-90 were simulated and compared to field data. The model successfully simulated solute transport for an unreactive conservative solute chloride, a solute with a first-order irreversible rate reaction, radioactive decay, and a solute with equilibrium-controlled ion exchange.

The program incorporated generalized expressions to treat dispersion as a tensor with both longitudinal and transverse components.

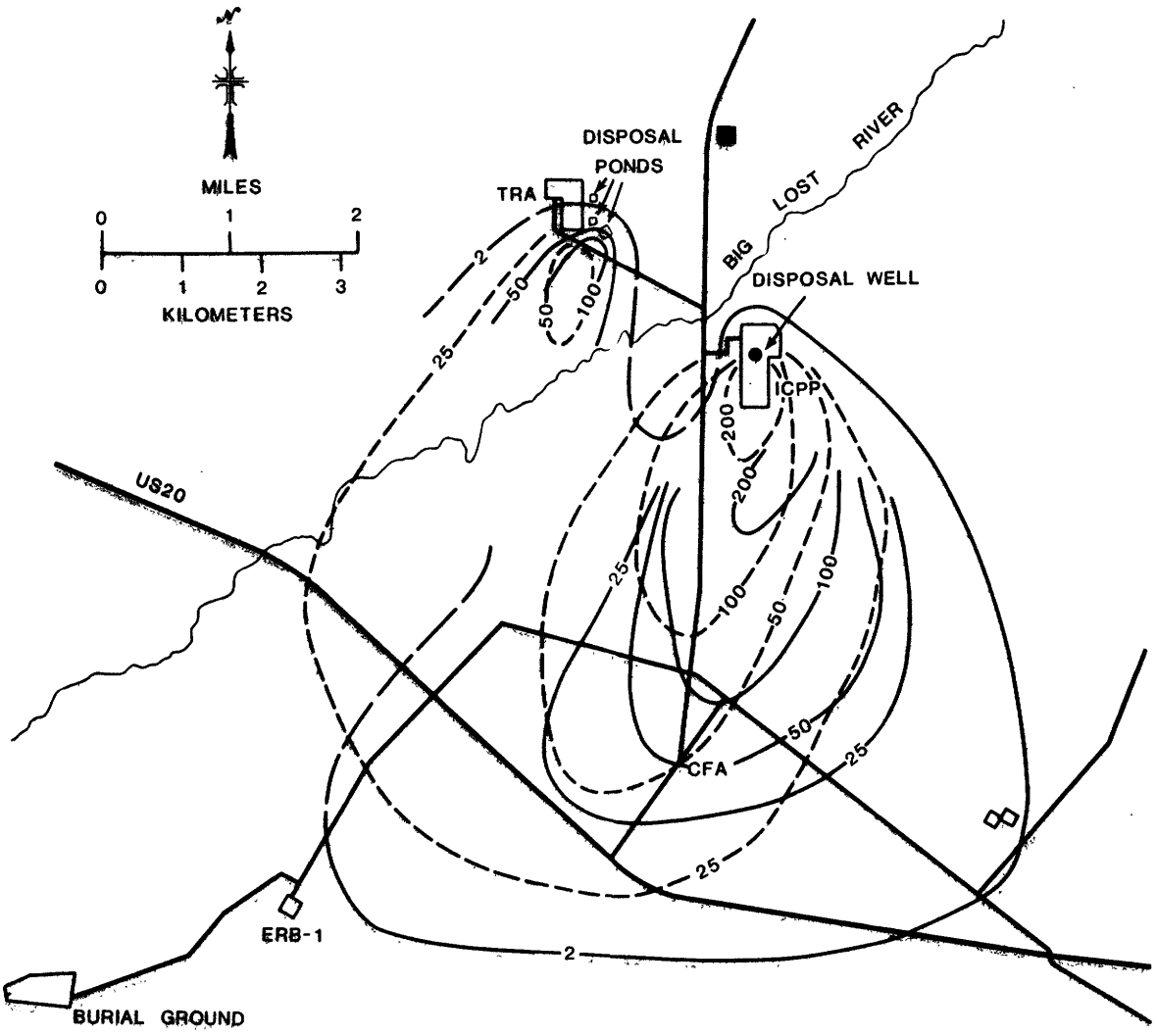
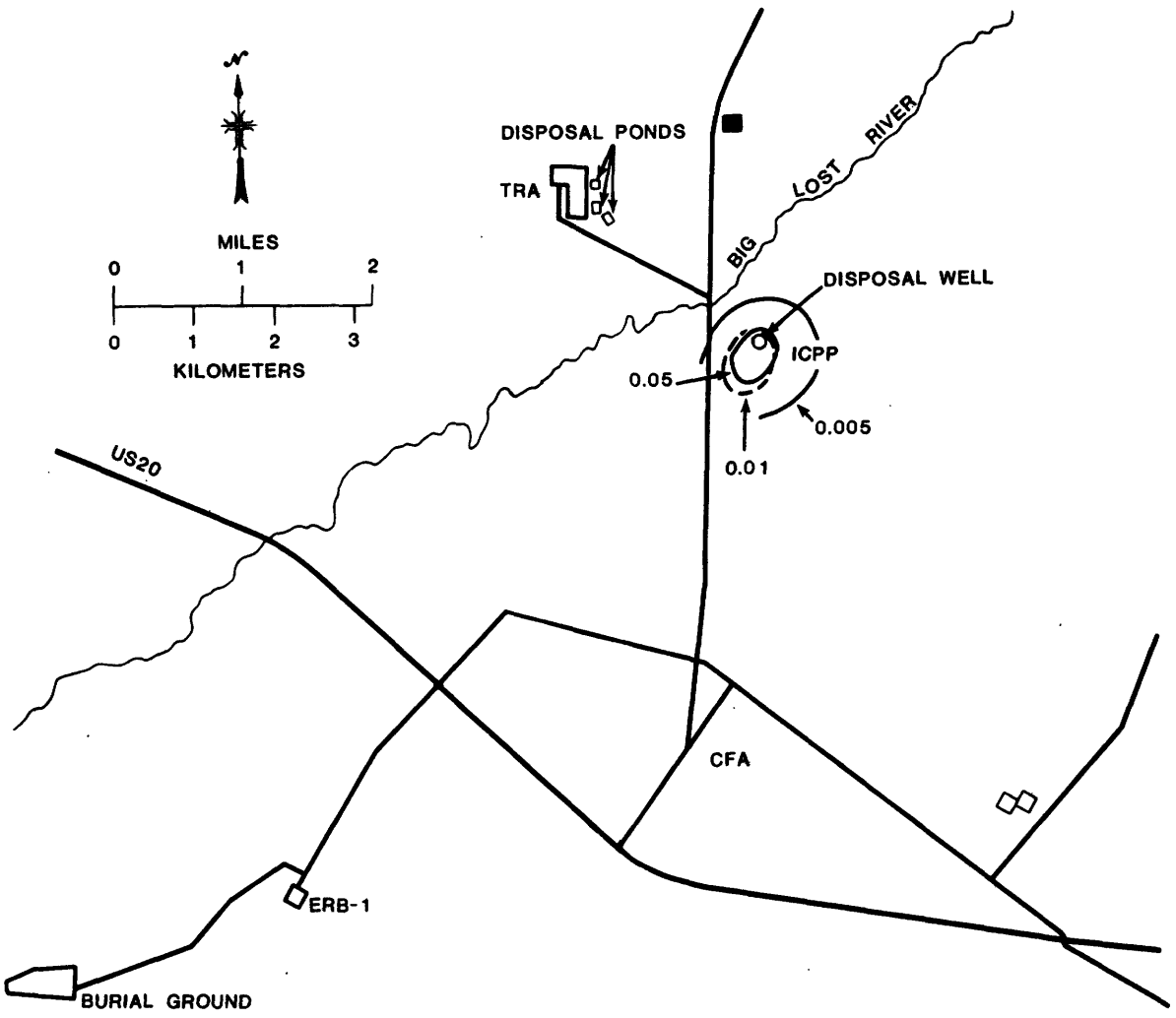


Figure 13.--*Comparison of waste tritium plumes for 1968-69 based on well sample data and computer model.*



EXPLANATION

EQUAL STRONTIUM 90 CONCENTRATION IN pCi/mL FOR 1964

———— 0.01 WELL SAMPLES

— — — — 0.01 DIGITAL MODEL (FINITE ELEMENT)

Figure 14.--*Comparison of waste strontium-90 plumes for 1964 based on well sample data and computer model.*

Previous studies using finite-difference methods to solve these same sets of transport equations showed the finite-element methods to be superior for large grid spacings. For the models presented here, the linear functions are superior to cubic functions for large two-dimensional problems.

As with any numerical technique, further study may reveal shortcuts or improvements to enhance the technique's features. The most productive research in this area would perhaps be a search for more efficient matrix-solution techniques for such sparce unsymmetric systems.

LITERATURE CITED

Aris, Rutherford, 1969, Elementary chemical reactor analysis: Englewood Cliffs, N.J., Prentice-Hall, 352 p.

Bear, Jacob, 1972, Dynamics of fluids in porous media: New York, American Elsevier, 764 p.

Bird, R. B., Steward, W. E., and Lightfoot, E. N., 1966, Transport phenomena: New York, John Wiley and Sons, 780 p.

Bolt, G. H., 1967, Cation exchange equations in soil science: A review, Jour. Agr. Sci., v. 15, p. 81-103.

Bredehoeft, J. D. and Pinder, G. F., 1973, Mass transport in flowing ground water: Water Resources Research, v. 9, no. 1, p. 194-209.

Brenner, Howard, 1962, The diffusion model of longitudinal mixing in beds of finite length. Numerical values: Chem. Eng. Sci., v. 17, p. 229-243.

Carnahan, B., Luther, H. A., and Wilkes, J. O., 1969, Applied numerical methods: New York, John Wiley and Sons, 604 p.

Cavendish, J. C., Price, H. S., and Varga, R. S., 1969, Galerkin methods for the numerical solution of boundary value problems: Petroleum Eng. Soc. Jour., June, p. 204-220.

Crandall, S. H., 1956, Engineering analysis, a survey of numerical Procedures: New York, McGraw Hill, p. 147-154.

Douglas, J., Jr. and Dupont, T., 1970, Galerkin methods for parabolic equations: Indus. and Appl. Math. Soc. Jour. Numerical Analysis, v. 7, no. 4, p. 575-626.

Finlayson, B. A., 1969, Applications of the method of weighted residuals and variational methods: British Chem. Eng., v. 14, no. 1, p. 53-57.

_____, 1972, The method of weighted residuals and variational principles: New York, Academic Press, 412 p.

Finlayson, B. A. and Scriven, L. E., 1965, The method of weighted residuals and its relation to certain variational principles for the analysis of transport processes: Chem. Eng. Sci., v. 20, p. 395-404.

Forray, M. J., 1968, Variational calculus in science and engineering: New York, McGraw Hill, 221 p.

Garder, A. O., Peaceman, D. W., and Pozzi, A. L., 1964, Numerical calculation of multidimensional displacement by the method of characteristics: Petroleum Eng. Soc. Jour., v. 4, no. 1, p. 26-36.

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

Harleman, D. R. F. and Rumer, R. R., Jr., 1963, Longitudinal and lateral dispersion in an isotropic porous medium: Fluid Mechanics Jour., v. 16, pt. 3, p. 385-394.

Harlow, F. H. and Amsden, A. A., 1970, Fluid dynamics: An introductory text: Los Alamos Scientific Laboratory of Calif., 90 p.

Helfferich, Friedrich, 1962, Ion exchange: New York, McGraw Hill, 624 p.

Hughes, J. L. and Robson, S. G., 1973, Effects of waste percolation of ground water in alluvium near Barstow, California in Underground waste mangement and artificial recharge: v. 1, p. 91-129.

IBM Corporation, 1968, IBM Application Program - System 1360 Scientific Subroutine Package Version III Programmers Manual, Program Number 360A-CM-03X, 454 p.

Keller, Herbert B., 1967, The numerical solution of parabolic partial differential equations, in Mathematical methods for digital computers, v. 1: New York, John Wiley and Sons, 293 p.

Konikow, L. F., and Bredehoeft, J. D., 1974, Modeling flow and chemical quality changes in an irrigated stream-aquifer system: Water Resources Research, v. 10, no. 3, p. 546-562.

Kreyszig, Erwin, 1962, Advanced engineering mathematics: New York, John Wiley and 856 p.

Krylov, V. I., 1962, Approximate calculation of integrals: translated by Authur H. Stroud: New York, The MacMillian Co., 355 p.

Lantz, R. B., 1970a, Quantitative evaluation of numerical diffusion (truncation error): Presented at Soc. Petroleum Engineers second numerical simulation symposium, Dallas, Texas, paper SPE 2811.

_____, 1970b, Rigorous calculation of miscible displacement using immiscible reservoir simulators: Soc. Petroleum Eng. Jour., June, p. 192-203.

Levenspiel, Octave, 1967, Chemical reaction engineering: New York, John Wiley and Sons, 501 p.

Longwell, P. A., 1966, Mechanics of fluid flow: New York, McGraw-Hill, 433 p.

Manteuffel, T. A., 1975, An iterative method for solving nonsymmetric linear systems with dynamic estimation of parameters: Dept. Computer Sci., Univ. Illinois, Urbana, 185 p.

Nalluswami, 1971, Numerical simulation of general hydrodynamic dispersion in porous medium: Ph. D. dissertation, Colorado State Univ., Fort Collins, 138 p.

Nalluswami, Marappagounder, Logenbough, R. A., and Sunada, D. K., 1972, Finite-element method for the hydrodynamic dispersion equation with mixed partial derivatives: Water Resources Research, v. 8, no. 3, p. 1247-1250.

Ogata, A. and Banks, R. B., 1961, A solution of the differential equation of longitudinal dispersion in porous media: U.S. Geological Survey Prof. Paper 411-A, 7 p.

Peaceman, D. W. and Rachford, H. H., Jr., 1962, Numerical calculation of multidimensional miscible displacement: Soc. Petroleum Engineers Jour., v. 2, no. 4, p. 327-339.

Pinder, G. F., 1973, A. Galerkin finite-element simulation of ground-water contamination on Long Island, New York: Water Resources Research, v. 9, no. 6, p. 1657-1670.

Pinder, G. F. and Cooper, Hilton, 1970, A numerical technique for calculating the transient position of the salt water front: Water Resources Reasearch, v. 6, no. 3, p. 875-882.

Pinder, G. F., and Frind, E. O., and Papadopulos, S. S., 1973, Functional coefficients in the analysis of ground-water flow: Water Resources Research, v. 9, no. 1, p. 222-226.

Price, H. S., Cavendish, J. C., and Varga, R. S., 1968, Numerical methods of higher order accuracy for diffusion-convection equations: Soc. Petroleum Engineers Jour., v. 8, p. 293-303.

Reddell, D. L. and Sunada, D. K., 1970, Numerical simulation of dispersion in ground-water aquifers: Colorado State Univ. Hydrology Paper 41, Fort Collins, 79 p.

Remson, I., Hornberger, G. M., and Molz, F. J., 1971, Numerical methods in subsurface hydrology: New York, Wiley Interscience, 389 p.

Robertson, J. B., 1974, Digital modeling of radioactive and chemical waste in the Snake River Plain Aquifer at the National Reactor Testing station, Idaho: U.S. Geol. Survey open-file rept., 41 p.

Robertson, J. B. and Barraclough, J. T., 1973, Radioactive and chemical-waste transport in ground water at National Reactor Testing Station, Idaho, 20-year case history, in Underground waste management and artificial recharge: Internat. Symposium on Underground Waste Management and Artificial Recharge, New Orleans, La., Sept. 26-30, 1973, Proc., issued by Am. Assoc. Petroleum Geologists, v. 1, p. 291-322.

Robertson, J. B., Schoen, Robert, and Barraclough, J. T., 1974, The influence of liquid waste disposal on the geochemistry of water at the National Reactor Testing Station, Idaho, 1952-70: U.S. Geol. Survey open-file rept., 231 p.

Rubin, J. and James, R. V., 1973, Dispersion-affected transport of solutes in porous media; I. The Galerkin method applied to equilibrium-controlled exchange in unidirectional, steady, saturated waterflow: Water Resources Research, v. 9, no. 5, p. 1332-1357.

Schechter, R. S., 1967, The variational method in engineering: New York, McGraw Hill, 287 p.

Scheidegger, A. E., 1961, General theory of dispersion in porous media: Jour. Geophys. Research, v. 66, no. 10, p. 3273-3278.

Shamir, U. Y. and Harleman, D. R. F., 1967, Numerical solutions for dispersion in porous mediums: Water Resources Research, v. 3, no. 2, p. 557-581.

Smith, G. D., 1965, Numerical Solutions of partial differential equations: New York, Oxford University Press, 179 p.

Snyder, L. J., Spriggs, T. W., and Stewart, W. E., 1964, Solution of the equations of change by Galerkin's method: Am. Inst. Chem. Eng. Jour., v. 10, no. 4, p. 535-540.

Wylie, C. R., Jr., 1966, Advanced engineering mathematics: New York, McGraw-Hill, 813 p.

Zienkewicz, O. C., 1971, The finite element method in engineering science: London, McGraw Hill, 521 p.