

**Solute Transport in Groundwater Under Density-Dependent Flow Conditions:
Development and Verification of a New Finite-Element Model**

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ABSTRACT

A simulation model is developed for prediction of the location, extent and severity of naturally occurring saltwater intrusion into freshwater aquifers under miscible-flow environments. The governing equations of flow in such systems include the equations of fluid continuity, Darcy velocity, solute-mass continuity and a state equation which relates fluid density to the solute concentration. The solution of this nonlinear set of equations was obtained here with the use of an iterative Galerkin finite-element scheme. The mixed formulation of the fluid-continuity and Darcy velocity equations resulted in a coupled set of approximate linear equations which were, then, decomposed into two sets of equations to be solved, sequentially, for pressure and velocity components. The mixed formulation provides a continuous approximation of the velocity field which is essential in preserving the solute-mass continuity across the boundary of the elements. Subsequent to the calculation of velocities, the solute-transport equation was solved with the use of a standard Galerkin finite-element method. In an application to the Henry's sea-water intrusion problem, the model developed based on the proposed formulation was shown to be accurate and efficient. Several features of the model, such as the storage and retrieval of the values of basis functions and their derivatives at Gauss-integration points, have eliminated the repetitive calculation of these terms needed for numerical integrations over elements; as a result they have increased the computational efficiency and practical applicability of the model.

INTRODUCTION

The contact of freshwater and saltwater is generally associated with the formation of complicated physiochemical processes, the complete description of which may not be mathematically tractable. To reduce complexity of the problem most investigators have regarded freshwater and saltwater as immiscible fluids separated by a sharp interface. However, in reality, a distinct interface does not exist between freshwater and saltwater, mainly, because the two fluids are miscible and there is only a slight difference in their densities. In fact, the two fluids become mixed and distributed in a dispersive zone of variable salinity.

Cooper (1959) was among the first to explain the mixing (or the dispersion zone) and the associated perpetual circulation of sea water in coastal aquifers. According to his hypothesis, the wedge front of the saltwater flowing inland is continuously being eroded by a seaward flow of mixed water in the zone of dispersion. This flow tends to reduce the extent to which saltwater may occupy the aquifer. Field investigation of Kohout (1964) verified Cooper's concept and confirmed the existence of the circulation phenomena along the Biscayne aquifer in the coastal region of Florida.

In corroboration of Cooper's hypothesis, Henry (1964) developed the first analytical solution of the effects of dispersion and density-dependent flow on saltwater encroachment in aquifers. Although by that time it had been discovered the magnitude of dispersion perpendicular to the velocity was much smaller than that in the direction of velocity, Henry (1964) assumed a constant-dispersion mechanism. Despite this and several other simplifying assumptions, the results of Henry's work clarified certain significant consequences of dispersion which until then had been inferred only on a qualitative

basis. Henry's quantitative description of dispersion phenomena set the stage for future investigations along this line.

With the advancement in computers, a series of more rigorous solutions of sea-water intrusion problems were obtained using a variety of numerical techniques. Among these studies is the work of Pinder and Cooper (1970), who used the method of characteristics in conjunction with an iterative ADI (Alternating Direction Implicit) procedure. Their approach was of practical importance in that it was applicable to heterogeneous, anisotropic aquifers with irregular geometry and different types of boundary conditions. Pinder and Cooper (1970) obtained a transient solution to the same example analyzed by Henry (1964). Their solution was shown to approach Henry's steady-state solution after passage of a long simulation time. Reformulating the problem in terms of stream functions, Lee and Cheng (1974) derived a steady-state solution for Henry's example using finite elements. Their solution, however, encountered convergence difficulty when advective transport was predominant. This latter formulation was shown by Huyakorn and Taylor (1976) to be inferior to a formulation based on pressure (or head) and salt concentration.

Segol et al. (1975) and Segol and Pinder (1976) were the first to develop a transient solution of the saltwater-encroachment problem on the basis of velocity-dependent dispersion coefficients. Using the mixed finite-element formulation of groundwater flow and Darcy velocity equations, they obtained accurate estimates of velocity components while preserving continuity of the velocity field across elemental boundaries. In advection-dominated transport problems, such a formulation is essential to achieving realistic solutions. A disadvantage associated with this approach is the need of solving a very large system of equations which increases the computational cost. For large aquifer-

fers requiring a long-term transient response, this disadvantage can limit the practical applicability of the mixed formulation.

With emphasis on optimum efficiency, Frind (1982a) has developed a finite-element model for simulation of saltwater intrusion that was found to be much less costly than comparable existing models. Two distinctive features of Frind's model are the elimination of static pressures in the fluid-flow equation, achieved by introduction of equivalent freshwater head, and the elimination of numerical integrations over elements, achieved by the deliberate choice of linear rectangular elements. Although this approach does not retain the continuity of the velocity field at the elemental boundaries, its solution was shown to approach that obtained with a continuous velocity as the grid size was refined. Frind (1982b) demonstrated that his model was capable of handling large simulation periods in aquifer systems of practical importance.

As indicated above, a variety of mathematical models are available for description of saltwater/freshwater systems. The specific conditions of the problem being analyzed determine the selection of an appropriate model. If the flow domain and boundary conditions are relatively simple and the aquifer has homogeneous characteristics, an analytical solution such as the one developed by Henry (1964) may well be sufficient. However, because of the hydrogeologic complexity involved, the majority of aquifer problems of practical interest necessitate the use of a sophisticated numerical model. Among various numerical models that are currently available for this use, a miscible-flow model based on the mixed formulation of the fluid-continuity and Darcy velocity equations results in the most accurate numerical solution of a freshwater/saltwater system but also suffers from lack of efficiency. In this study, it will be shown, however, that with careful construction of the

approximate equations, the efficiency of computations can be increased considerably without any loss in accuracy.

GOVERNING EQUATIONS

The distribution of solute (salt) concentration in a freshwater/saltwater system can be obtained by simultaneous solution of the coupled equations of fluid continuity, Darcy velocity and solute-mass continuity. The general form of these equations for two-dimensional cross sectional flow is expressed as

$$\text{fluid continuity, } \frac{\partial}{\partial x_i} (q_i) = 0 \quad (1)$$

$$\text{Darcy velocity, } q_i = - \frac{k_{ij}}{\mu} \left(\frac{\partial p}{\partial x_j} + \rho g_j \right) \quad (2)$$

$$\text{solute transport, } \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (q_i c / \theta) = \frac{\partial c}{\partial t} \quad (3)$$

where c represents the solute concentration, p is the pressure, q_i is the component of Darcy velocity in i -direction, ρ represents the fluid density, k_{ij} 's are components of the permeability tensor, D_{ij} 's are components of the dispersion coefficient tensor, g_j is the component of gravitational vector in j -direction, μ is the fluid viscosity, θ is the effective porosity, x_i ($i = 1, 2$) are the Cartesian coordinates, and t is the time variable. In derivation of the fluid-balance equation (1), the release of water from storage is assumed to have a negligible effect on movement of the saltwater front. We have also assumed that porosity, θ , and dynamic viscosity, μ , are constant in time and space.

So far we have introduced four unknowns; i.e. ρ , q_i , p and c , but only

three equations. The additional equation required for solution of these equations is a relationship between fluid density and salt concentration. Such a relationship is obtained by writing the first order Taylor expansions of fluid density about a base density and concentration:

$$\rho = \rho(c) \approx \rho_b + \frac{\partial \rho}{\partial c} (c - c_b) \quad (4)$$

where ρ_b is the base fluid density at base-concentration c_b (the base condition is usually taken as that of freshwater in which case $\rho_b =$ density of freshwater and $c_b = 0$) and $\frac{\partial \rho}{\partial c}$ is a constant value, representing the rate of changes in density with concentration which is obtained empirically.

Solution of equations (1) through (4) requires additional information in the form of initial and boundary conditions. As initial condition we must be given the salt concentration at some initial time, t_0 , at all spatial points, that is

$$c(x_i; t = t_0) = c_0(x_i) \quad \text{for } x_i \in R \quad (5)$$

where R indicates the spatial domain and c_0 is a known function. c_0 is used as a starting point to find the transient variations in solute concentration. The initial pressure distribution is not needed due to the elimination of the transient storage term in equation (1). In other words, the propagation of pressure has been assumed to be instantaneous. However, the pressure can change temporally because of the changes in fluid density.

The boundary conditions associated with the groundwater flow equations (1) and (2) may be of either the prescribed pressure type or the prescribed flux type. The prescribed pressure boundary condition requires that the

pressure distribution at points along the boundary segment, B_1 , remain the same as certain prespecified values, i.e.

$$p(x_1, t) = p_B(x_1, t) \quad \text{for } x_1 \in B_1, t > t_0 \quad (6a)$$

where P_B represents a given pressure distribution. This type of boundary condition is usually used as a far-field boundary where no appreciable change in piezometric surface is expected to take place.

The prescribed flux condition specifies the flux normal to the boundary segment B_2 as

$$q(x_1, t) = q_n(x_1, t) \quad \text{for } x_1 \in B_2, t > t_0 \quad (6b)$$

where q_n is the specified Darcy flux. $B = B_1 + B_2$ is the total boundary of the spatial domain. An impermeable boundary is a special case of prescribed flux boundary conditions. In the case of leakage through a semipervious boundary, the normal flux can be evaluated in terms of the equivalent fresh-water head differential and the material properties of the leaky layer (Frind, 1982b).

As is obvious from equations (6a) and (6b), the boundary conditions of groundwater flow can be time-dependent. However, the transient variations of the boundary-pressure and boundary-flux terms are usually assumed insignificant for most practical situations.

In obtaining the solution of the solute-transport equation (3), the boundary conditions must be specified for all time periods. The types of conditions which are commonly encountered in actual field problems include the

conditions of prescribed concentration and a more complicated form of prescribed flux. The prescribed-concentration distribution is usually given in the form of

$$c(x_i, t) = c_B(x_i, t) \quad \text{for } x_i \in B_3, t > t_0 \quad (7a)$$

where c_B is the functional form of a specified concentration. The prescribed flux-condition (also known as the Cauchy condition) is expressed by

$$\left(\frac{q_i}{\theta} c - D_{ij} \frac{\partial c}{\partial x_j} \right) n_i = \frac{q_n}{\theta} c_n \quad \text{for } x_i \in B_4, t > t_0 \quad (7b)$$

where n_i is the i -th component of the outward unit vector normal to the boundary, c_n is the concentration of the inflowing fluid through the boundary and $B = B_3 + B_4$ is again the spatial-aquifer boundary. Equation (7b) is usually used in the case of an inflow boundary when the rate and concentration of the entering fluid, q_n and c_n , are given. If flow is leaving the boundary, q_n and c_n are unknown. In such case the advective flux normal to the boundary is assumed to remain the same on both sides of the boundary. As a result of this, the boundary condition (7b) transforms into the Neumann-type boundary conditions of the form:

$$\frac{\partial c}{\partial n} = 0 \quad \text{for } x_i \in B_4, t > t_0 \quad (7c)$$

Equation (7c) also applies to an impermeable boundary in which case the normal flux, q_n , becomes zero.

With the specification of the governing equations along with the initial and boundary conditions, the mathematical description of a miscible-flow

system is complete. The system of equations (1) through (4) are coupled by the fact that the solution of the solute-transport equation (3) requires an appropriate representation of velocity field which depends on the fluid density which, in turn, is evaluated on the basis of solute concentration. The solution of such a complex nonlinear system of equations can be obtained with an iterative numerical scheme and this will be described in the subsequent section.

GALERKIN FINITE-ELEMENT SOLUTION

Quite frequently, the numerical solution of the governing equations (1) and (2) is carried out by first writing the fluid-continuity equation in terms of pressure incorporating the equations for velocity. The pressure distribution obtained from solution of the resulting equation is then used in the set of equations for velocity to determine the Darcy velocity components. For situations characterized by smooth variations of pressure, this approach indeed has been proven to be quite effective requiring minimal computational efforts. The inherent difficulty associated with this approach is, however, a discontinuity in the velocity field across the inter-elemental boundaries when zero-order continuous-basis functions are used to represent the pressure (Pinder and Gray, 1977). When using these velocities for solution of the solute-transport equation (3), the discontinuity in velocity leads to a violation of mass conservation in a local sense. This lack of continuity can distort the solution of the solute-transport equation for advective-dominated transport problems.

In an attempt to achieve a continuous-velocity field, Meissner (1973) suggested a mixed formulation for solving the fluid continuity and Darcy

velocity equations simultaneously. This approach leads directly to the nodal values of pressure and velocity. As indicated before, Segol et al. (1975) used the mixed finite-element formulation within the context of a saltwater-intrusion model. The results of their analysis showed a significant improvement but at the expense of a considerable increase in computations. Consequently very few future applications of this technique have been reported in the groundwater literature. The use of mixed finite-element method has received a great popularity in problems of fluid mechanics.

A mixed finite-element formulation is utilized here to solve the fluid continuity and Darcy velocity equations. Having obtained an appropriate velocity field, we then proceed to demonstrate the solution of the solute-transport equation using a standard Galerkin finite-element method.

Fluid Continuity and Darcy Velocity Equations

The first step in Galerkin formulation of the approximate equations is to assume a set of trial solutions of the form:

$$p(x,z,t) \approx \sum_{j=1}^m p_j(t) \phi_j(x,z) \quad (8a)$$

$$q_x(x,z,t) \approx \sum_{j=1}^n q_{xj}(t) \phi_j(x,z) \quad (8b)$$

$$q_z(x,z,t) \approx \sum_{j=1}^n q_{zj}(t) \phi_j(x,z) \quad (8c)$$

where $p_j(t)$, $q_{xj}(t)$ and $q_{zj}(t)$ are, respectively, the unknown nodal values of pressure, x-component of velocity and z-component of velocity; x and z are the Cartesian coordinates, ϕ_j and ϕ_j are an appropriate set of basis functions and m and n are respectively the number of nodes used for approximation of

pressure and velocity. Note that p , q_x and q_z are dependent on time due to the fact that the fluid density changes with concentration. The choice of basis functions, ϕ_j and ψ_j , are affected by the level of accuracy required. Optimum efficiency and accuracy are achieved only when the variation in pressure is approximated by basis functions of one order lower than those used for defining the velocity distributions (Huyakorn and Taylor, 1976). The common practice is to use quadrilateral elements with eight nodes to represent the velocity and then use only the corner nodes for approximating the pressure.

The differential operators associated with equations (1) and (2) are written as

$$L(q_x, q_z) = \frac{\partial}{\partial x} (q_x) + \frac{\partial}{\partial z} (q_z) = 0 \quad (9a)$$

$$L(q_x, p) = q_x + \frac{k_{xx}}{\mu} \left(\frac{\partial p}{\partial x} \right) = 0 \quad (9b)$$

$$L(q_z, p) = q_z + \frac{k_{zz}}{\mu} \left(\frac{\partial p}{\partial z} - \rho g \right) = 0 \quad (9c)$$

where, for simplicity, the two-dimensional x - z coordinate system is taken to be in the horizontal and vertically upward directions and it is further assumed that the x - z axes are colinear with the principal directions of the permeability tensor. As a result of this latter assumption, the terms involving $k_{xz} = k_{zx} = 0$ have been eliminated from equations (9b) and (9c). Note also from equation (9b) that the body-force term which has zero component in the horizontal direction, x , has been eliminated.

The next step is to substitute the trial solutions in equations (9a), (9b) and (9c); the residuals of the equations are subsequently multiplied by

the appropriate basis functions and are, then, integrated over the spatial domain. By the orthogonality condition of the Galerkin theory, the resulting set of algebraic equations must be set to zero. This operation will eventually lead to the following set of approximate equations to be solved for pressure and Darcy velocity components:

$$[K_x] \{q_x\} + [K_z] \{q_z\} = \{f_Q\} \quad (10a)$$

$$[M_x] \{q_x\} + [L_x] \{p\} = \{f_x\} \quad (10b)$$

$$[M_z] \{q_z\} + [L_z] \{p\} = \{f_z\} \quad (10c)$$

where $\{p\} = (p_1, p_2, \dots, p_m)^T$, $\{q_x\} = (q_{x1}, q_{x2}, \dots, q_{xn})^T$ and $\{q_z\} = (q_{z1}, q_{z2}, \dots, q_{zn})^T$ are vectors of unknown nodal variables; and the components of coefficient matrices K_x , K_z , L_x , L_z , M_x and M_z and the right-hand-side vectors f_Q , f_x and f_z are defined in Table 1. Incorporation of boundary conditions in the set of equations (10) is carried out simply by moving the terms including the known values of p_j , q_{xj} and q_{zj} to the right-hand sides. The equations corresponding to the nodes with prescribed-pressure and prescribed-flux conditions are subsequently eliminated from further analysis. The remaining set of equations ready to be solved will look very similar to (10) and will not be rewritten; however, to reflect the modification made by incorporation of boundary conditions, hereafter we use \bar{K}_x , \bar{K}_z , \bar{L}_x , \bar{M}_x and \bar{M}_z as coefficient matrices; \bar{f}_Q , \bar{f}_x and \bar{f}_z as right-hand-side vectors; and \bar{p} , \bar{q}_x and \bar{q}_z as unknown terms. Note that the dimensions of these terms are smaller than their original counterparts in the set of equations (10). Moreover, certain components of the right-hand-side vec-

tors that were previously zero, may now contain non-zero contributions of the boundary conditions.

The set of linear equations (10) or its modified version can be solved simultaneously as was shown by Segol et al. (1975). This approach, however, takes a considerable amount of computer time and storage. An alternative approach is to decompose the system into three separate equations to be solved for \bar{p} , \bar{q}_x and \bar{q}_z . The decomposition is carried out by elimination of \bar{q}_x and \bar{q}_z from equation (10a) using the relationship (10b) and (10c). The resulting set of equations to be solved for pressure is derived to be

$$[A] \{\bar{p}\} = \{Q\} \quad (11)$$

where $[A] = [\bar{K}_x] [\bar{M}_x]^{-1} [\bar{L}_x] + [\bar{K}_z] [\bar{M}_z]^{-1} [\bar{L}_z]$
and $\{Q\} = [\bar{K}_x] [\bar{M}_x]^{-1} \{\bar{f}_x\} + [\bar{K}_z] [\bar{M}_z]^{-1} \{\bar{f}_z\} - \{\bar{f}_Q\}.$

The pressure distribution, \bar{p} , calculated from equation (11) is substituted in the following equations for computation of velocity components:

$$[\bar{M}_x] \{\bar{q}_x\} = \{\bar{f}_x\} - [\bar{L}_x] \{\bar{p}\} \quad (12a)$$

$$[\bar{M}_z] \{\bar{q}_z\} = \{\bar{f}_z\} - [\bar{L}_z] \{\bar{p}\} \quad (12b)$$

The sets of equations (11) and (12) represent the final numerical approximation of the fluid-continuity and Darcy velocity equations. The solution process for these equations is sequential and starts by solving equation (11) for pressure and then proceeding to construct the right-hand sides of equations (12a) and (12b) and solving these equations for velocities. The

velocity values will be used in the numerical approximation of the solute-transport equation which is the subject of the next section.

Solute-transport Equation

The standard Galerkin finite-element approach is used for solution of the solute-transport equation (3). As mentioned before, at this stage of the solution process, the Darcy velocity components, q_x and q_z , are given from the solution of the groundwater flow equations. The values of velocities are used beforehand to determine the velocity-dependent components of the dispersion-coefficient tensor, D_{ij} , using the relationships given in Bear (1979). The advective-transport term in equation (3) is also dependent on the velocities, but this dependence is directly included in the subsequent numerical formulations.

Following an approach analogous to the previous section, we approximate the unknown solute concentration in terms of a trial solution of the form:

$$c(x,z,t) \approx \sum_{j=1}^n c_j(t) \phi_j(x,z) \quad (13)$$

where c_j 's represent the unknown nodal concentrations and ϕ_j 's are the basis functions that are selected as a matter of simplicity to be the same as the basis functions used for representation of velocity. The known components of the dispersion coefficient can also be expressed in the form of finite series, for example:

$$D_{xx}(x,z,t) \approx \sum_{j=1}^n D_{xxj}(t) \phi_j(x,z) \quad (14)$$

where D_{xxj} 's are the nodal dispersion values. Similar expressions can be written for D_{zz} , D_{xz} and D_{zx} . Note that the aquifer porosity, θ , is a constant.

The differential operator of the solute-transport equation (3) is written in its expanded form as

$$L(c) = \frac{\partial}{\partial x} (D_{xx} \frac{\partial c}{\partial x}) + \frac{\partial}{\partial x} (D_{xz} \frac{\partial c}{\partial z}) + \frac{\partial}{\partial z} (D_{zx} \frac{\partial c}{\partial x}) + \frac{\partial}{\partial z} (D_{zz} \frac{\partial c}{\partial z}) - \frac{\partial}{\partial x} (v_x c) - \frac{\partial}{\partial z} (v_z c) - \frac{\partial c}{\partial t} = 0 \quad (15)$$

where $v_x = q_x/\theta$ and $v_z = q_z/\theta$ are pore velocities.

Utilizing the Galerkin approach, the approximate integral equations are obtained by making the residual arising from substitution of equation (14) into (15) orthogonal to each of the basis functions, ψ_j . A set of ordinary differential equations will eventually result from this operation which, in matrix form, is expressed as

$$[S] \{c\} + [T] \left\{ \frac{dc}{dt} \right\} = [f] \quad (16)$$

where S is the advective-dispersive transport matrix, T is the solute-mass matrix and the right-hand-side vector f contains the dispersive-mass fluxes at the boundary. The typical elements of S , T and f are defined in Table 1. In formulating these equations, Green's theorem is applied to break up the second derivatives. Moreover, the components of the flux-derivatives resulting from expansion of the advective terms in equation (15), i.e. the terms involving $\partial v_x / \partial x$ and $\partial v_z / \partial z$, were assumed to be negligible and, therefore, were eli-

minated during the development of the approximate equations. This assumption is acceptable in the absence of fluid sources and sinks (Frind, 1982a). Note also that the boundary-flux term is non-zero only at an inflow boundary in which case it is evaluated with the use of equation (7b).

We can now proceed to solve the set of ordinary differential equations (16) by finite-difference time stepping. Employing a finite-difference approximation of the temporal derivatives, equation (16) can be written in a time-weighted form as

$$[M] \{c\}_{t+\Delta t} = [N] \{c\}_t + \{f_c\} \quad (17)$$

where the coefficient matrices M and N and the vector f_c are given by

$$[M] = w [S] + \frac{1}{\Delta t} [T] \quad (18a)$$

$$[N] = - (1 - w) [S] + \frac{1}{\Delta t} [T] \quad (18b)$$

$$\{f_c\} = w \{f\}_{t+\Delta t} + (1 - w) \{f\}_t \quad (18c)$$

in which $1/2 < w < 1$ is the time-weighting factor, and Δt represents the time interval. A value of $w = 1/2$ results in the Crank-Nicolson approximation which is second order accurate in time but occasionally produces oscillatory solutions. On the other hand, a value $w = 1$ (implicit scheme) provides good stability but may result in greater smearing of the solute distribution. Depending on the problem being analyzed, an appropriate choice of w can usually be obtained within a few trials.

Starting from some initial values, equation (17) will determine the transient variations in solute concentration. For advective-dominated transport problems, numerical difficulties in the form of artificial dispersion and overshooting may be encountered. An improved estimate of velocities as obtained in this study may alleviate some of these difficulties. Mesh refinement is known to reduce the tendency of overshooting. The upstream-weighted technique presented by Huyakorn and Nilkuha (1979) is another way of avoiding numerical dispersions but at the expense of smearing the concentration front.

Computational Framework

Because of the nonlinearity involved, equations (1), (2) and (3) or their numerical approximations, equations (11), (12) and (17), have to be solved in combination with equation (4) in an iterative manner. The solution procedure for each time step begins with an estimate of fluid density obtained from equation (4) using the concentration distribution from the previous time step. The coefficients in the equations for pressure and velocity, equations (11) and (12), are determined on the basis of this estimate of fluid density and then these equations are solved in a sequential approach. The nodal values of velocities obtained from solution of equation (12) are used to define the advective and dispersive components in equation (17). Subsequently, equation (17) is solved to yield the salt-concentration distribution. At this stage, the nodal values of the fluid density are updated using the new estimate of concentration in equation (4), and the whole cycle is repeated once more. This process continues until the successive concentration values are within a specified tolerance. At this stage we can proceed to perform the computations for the next time step.

The iterative process described above usually converges rather rapidly, provided the time interval is not too large. According to Frind (1982a), the choice of an appropriate time interval is controlled in most problems by the need to keep the numerical dispersion to an acceptable level rather than the convergence criteria. A time-lagged approach suggested by Segol et al. (1975) has also been shown to be very effective for long-term transient simulation of problems with densities lower than that of sea water. In this case, the elapsed time between solutions of the flow equations is much larger than the time interval for computation of solute concentration.

During the course of model development, care must be taken in reducing the computer-storage requirement and in increasing the computational efficiency. Considerable saving was achieved in our model by storing the computed values of the elemental-basis functions and their derivatives at the Gauss-integration points on an input/output file. Consequently, future reference to these values was obtained rather easily without the need to repeat any computation. The model takes full advantage of the specific structure of the coefficient matrices. For matrices \bar{M}_x and \bar{M}_z in equation (12) that are banded and symmetric, only the elements within the upper band-width are stored. The banded portions of the non-symmetric matrices \bar{K}_x , \bar{K}_z , \bar{L}_x , \bar{L}_z , M and N are retained in rectangular two-dimensional arrays. The construction of coefficient matrices in equations (11) and (12), i.e. A, \bar{M}_x and \bar{M}_z , are needed only once. At each time step only the right-hand-side vectors of these equations have to be updated. The coefficient matrix in equation (17), i.e. M, is reconstructed whenever the time interval, Δt , changes or the velocities are updated. Solution of the equations are carried out efficiently using a Gauss solver for equation (11), a Cholesky solver for equation (12) and a Gaussian routine for non-symmetric coefficient

matrices in equation (17).

NUMERICAL RESULTS

A computer model was developed on the basis of the formulation presented in this study. Here we demonstrate the usefulness of this model for simulation of variable-density flow problems.

The analytic solution to the example problem devised by Henry (1964) is usually used as a benchmark against which other solutions are compared. The problem involves the intrusion of saltwater into a confined coastal aquifer. The configuration of the vertical cross section of this aquifer is depicted in Figure 1. Inland freshwater recharges the aquifer from the left boundary while at the same time the denser sea water is moving inland from under the freshwater. At equilibrium a dispersive zone develops at the contact of the two fluids through which the mixed water circulates and returns back to the sea.

The aquifer is assumed to be homogeneous and isotropic. The dispersion coefficient is assumed constant although, in reality, it changes with variations in velocity. Initially, the aquifer is occupied only with freshwater. The prescribed flux and prescribed pressure-boundary conditions are assumed, respectively, along the left and right vertical boundaries. The upper and lower boundaries are impermeable. The hydrogeologic parameters associated with this problem are given in Table 2.

During the course of numerical experiments, approximations of pressure, p , velocity, v , and salt concentration, c , were obtained over the aquifer domain using three types of interpolation scheme: (1) linear interpolations for p , v and c (Figure 2-a); (2) quadratic interpolations for p , v and c

(Figure 2-b); and (3) mixed interpolations, i.e. quadratic interpolations for v and c (Figure 2-b) and linear interpolation for p (using corner nodes in Figure 2-b). The mixed-interpolation scheme, as indicated before, is expected to provide the most accurate solution among the three schemes.

The first analysis was performed to check the accuracy of the model results using only the mixed-interpolation scheme. The computed 0.5 isochlor from the present model is displayed in Figure 3 with the similar contour lines from the steady-state solution of Henry (1964), the transient solution of Segol et al. (1975) and the transient solution obtained from using the U.S. Geological Survey "SUTRA" model (Voss, 1984). The comparison of our transient solutions for the elapsed time of 30 and 100 minutes with the solutions obtained by Segol et al. (1975) and SUTRA is excellent (see Figure 3). For the most part, the three sets of isochlors are located in close proximity to each other. One interesting observation is that due to the existence of artificial vertical velocities along the right boundary in the Segol et al. formulation, the top portion of the dispersive zone tends to be narrow and the tip of the saltwater zone calculated by their model stays slightly higher than that determined by our model. This difficulty was removed in our analysis by explicitly setting these velocities to zero.

To obtain the steady-state solution, the simulation time was extended to 500 minutes. After the elapsed time of 300 minutes, the top portion of the dispersive zone remained relatively stable while the bottom portion moved only slightly. The 0.5-isochlor line for the 300-minute time period shown in Figure 3 can be considered to be representative of the quasi-steady-state solution of Henry's problem. Again the agreement between Henry's solution and the model results is reasonably good. The calculated 0.5-isochlor line also

matched quite well with the results of SUTRA model for the elapsed time of 300 minutes.

Figure 3 also depicts the Ghyben-Herzberg interface obtained based on the assumption of immiscible-fluid flows (Henry, 1964). An important observation is the extensive location of the saltwater toe which obviously overestimates reality by as far as twice the actual distance. This is a good indication of inappropriateness of sharp-interface models for situations characterized by significant dispersion. This point is clarified even further in Figure 4 where the whole spectrum of the dispersive zone is demonstrated for the elapsed time of 300 minutes. Note again the large extent of the top portion of the dispersive zone created by removal of artificial vertical velocities.

The transient changes in solute-concentration distribution along the bottom of the aquifer are depicted in Figure 5. As can be seen, the dispersive zone starting from a relatively narrow strip has gradually extended over a large portion of the aquifer. The changes in solute concentration have, almost, been stabilized after the 100-minute elapsed time.

To gain insight into the hydrodynamics of the flow in a density-dependent system, the nodal velocities were plotted in Figure 6 for the elapsed time of 300 minutes. As seen in Figure 6, the vertical components of velocities within the saltwater-freshwater mixing zone were affected significantly by the variations in density. The changes in velocities become less important during latter time steps. In most problems, after reaching a certain quasi-stabilization point in time, the changes in vertical velocities are minimal and in fact the calculation of velocities can be carried out much less frequently than that of salt concentration. In our analysis we updated the velocities at all time steps although it could have been avoided. The

velocity vectors demonstrate clearly the whole circulation process of the saltwater-intrusion phenomenon.

The last experiment involved using all three different interpolation schemes for solution of Henry's problem. The 0.5 isochlors obtained for the elapsed time of 30 and 100 minutes are depicted in Figure 7. The toe of the isochlor from the linear-interpolation scheme is extended further inland while that from the quadratic-interpolation scheme is sharper and shorter. The isochlors calculated with mixed interpolations are smooth and for the most part are in close agreement with the solution from the linear interpolation scheme. However, it is not clear why the solution obtained with the use of quadratic-interpolation scheme deviates considerably from that obtained using linear- or mixed-interpolation scheme for long simulation times.

SUMMARY AND CONCLUSIONS

A finite-element model was developed for sequential solution of the fluid continuity, Darcy velocity and solute-transport equations. The model, while preserving the continuity of the velocity field, results in accurate approximation of the velocity field which is essential in the analysis of miscible-flow problems. Several other features of the model such as the storage of basis functions and their derivatives at Gauss-integration points on an input-output file have improved the efficiency of the computations substantially.

In an application to the Henry's sea-water intrusion problem, the model was shown to reach a state of dynamic equilibrium with minimal computational efforts. The high accuracy of the model results was demonstrated through excellent comparisons with several available solutions. We have also shown

that substantial errors will occur if a sharp-interface model is used to simulate a saltwater intrusion problem involving significant dispersion. Indeed, in most practical situations, the use of a miscible flow model is essential to achieving realistic solutions.

While different types of interpolation functions can be used in the proposed finite-element model, we suggest to approximate the velocity and concentration with isoparametric quadrilateral elements containing eight nodes but then use only the four corner nodes for bilinear approximation of pressure.

The proposed model can be easily modified to accommodate three-dimensional flows or leakage through a second layer. This will obviously require additional computational work and further measures to increase the efficiency may be needed.

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Table 1. List of equations describing the different components of coefficient matrices and vectors and their specific characteristics.

Matrix or Vector	Typical Component	Dimension	Specific Characteristics
K_x	$\int_R \frac{\partial}{\partial x} (\phi_j) \phi_i \, dR$	$n \times n$	banded, non-symmetric
K_z	$\int_R \frac{\partial}{\partial z} (\phi_j) \phi_i \, dR$	$n \times n$	banded, non-symmetric
L_x	$\int_R \left(\frac{k_{xx}}{\mu} \right) \frac{\partial}{\partial x} (\phi_j) \phi_i \, dR$	$n \times n$	banded, non-symmetric
L_z	$\int_R \left(\frac{k_{zz}}{\mu} \right) \frac{\partial}{\partial z} (\phi_j) \phi_i \, dR$	$n \times n$	banded, non-symmetric
M_x or M_z	$\int_R \phi_j \phi_i \, dR$	$n \times n$	banded, symmetric
f_Q	0	$n \times 1$	---
f_x	0	$n \times 1$	---
f_z	$\int_R \left(\frac{k_{zz}}{\mu} \right) \left[\sum_{k=1}^n \rho_k \phi_k \right] \phi_i \, dR$	$n \times 1$	---
S	$\int_R \sum_{k=1}^n \left\{ D_{xxk} \phi_k \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} + D_{xzk} \phi_k \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial z} \right.$ $+ D_{zxk} \phi_k \frac{\partial \phi_j}{\partial z} \frac{\partial \phi_i}{\partial x} + D_{zzk} \phi_k \frac{\partial \phi_j}{\partial z} \frac{\partial \phi_i}{\partial z}$ $\left. + v_{xk} \phi_k \frac{\partial \phi_j}{\partial x} \phi_i + v_{zk} \phi_k \frac{\partial \phi_j}{\partial z} \phi_i \right\} dR$	$n \times n$	banded, non-symmetric
T	$\int_R \phi_j \phi_i \, dR$	$n \times n$	banded, symmetric
f	$\int_B \left(D \frac{\partial c}{\partial n} \right) \phi_i \, dB$	$n \times 1$	---

Table 2. Values of physical parameters for Henry's problem

Parameter	Value
aquifer porosity	$\theta = 0.35$
hydraulic permeability	$k = 1.020408 \times 10^{-9} \text{ m}^2$
fluid viscosity	$\mu = 10^{-3} \text{ kg}/(\text{msec})$
dispersion coefficient	$D = 6.6 \times 10^{-6} \text{ m}^2/\text{sec}$
left-boundary influx velocity	$v = 6.6 \times 10^{-5}/0.35 = 1.885 \times 10^{-4} \text{ m}/\text{sec}$
right-boundary pressure distribution	$p_B = \rho_s g (\text{depth})$
sea-water density	$\rho_s = 1025 \text{ kg}/\text{m}^3$
freshwater density	$\rho_f = 1000 \text{ kg}/\text{m}^3$
sea-water salt concentration	$c_s = 0.0357 \text{ kg (dissolved solids)}/\text{kg (sea water)}$
acceleration of gravity	$g = 9.8 \text{ m}/\text{sec}^2$
constant rate of changes in density with concentration	$\frac{\partial \rho}{\partial c} = 700 \frac{\text{kg}(\text{sea water})^2}{\text{kg}(\text{total dissolved solids}) \text{ m}^3}$
aquifer thickness	$d = 1.0 \text{ m}$
aquifer length	$l = 2.0 \text{ m}$

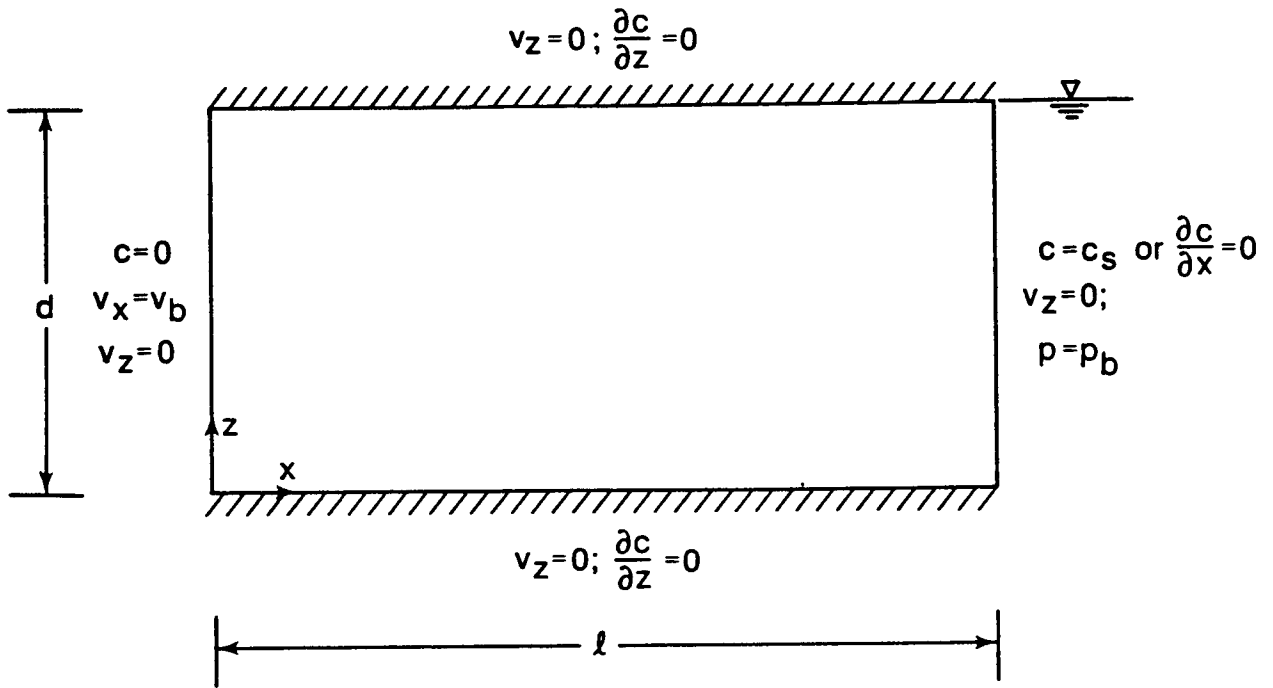
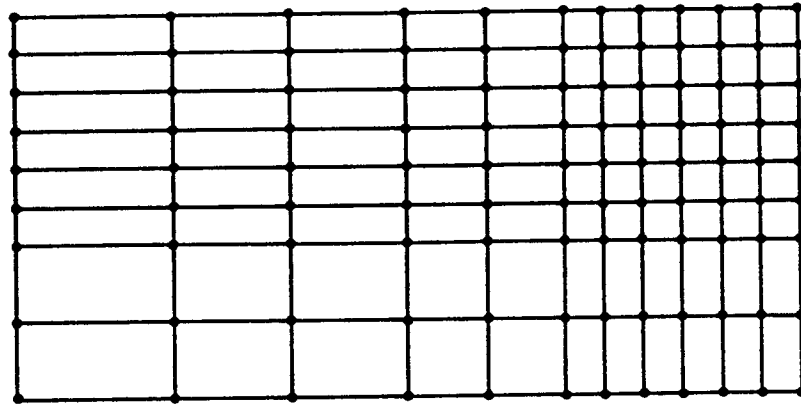
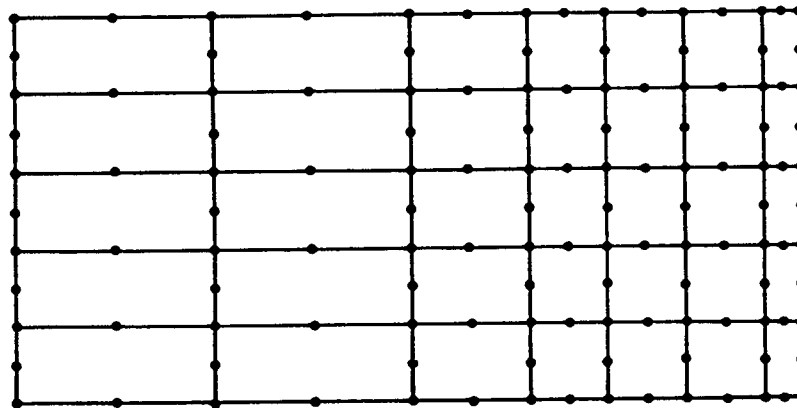


Figure 1. Schematic Representation of the Henry's Example



(a) linear elements



(b) quadratic elements

Figure 2. Finite-Element Discretization of the Aquifer Domain for the Henry's Problem

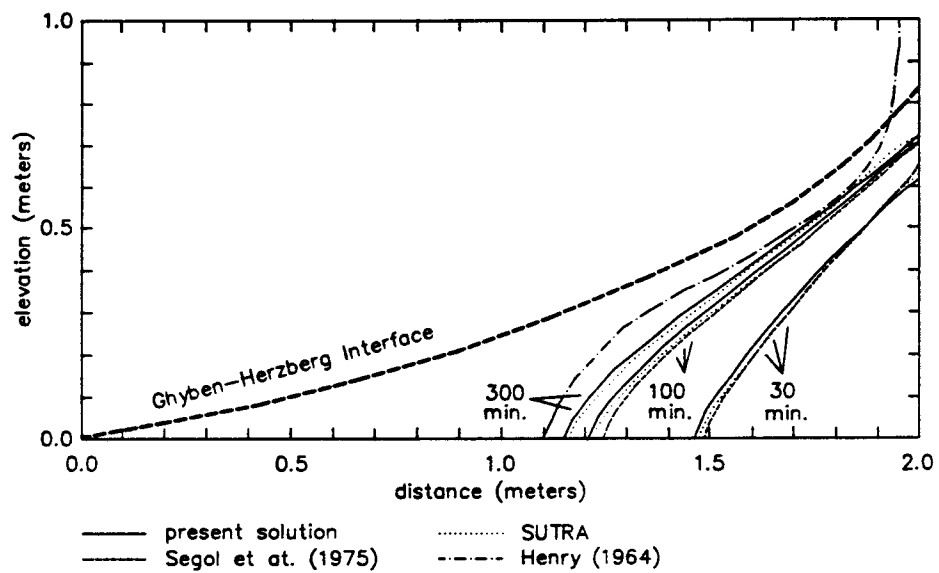


Figure 3. The Comparison of 0.5 Isochlors Computed by the Present Model Using Mixed Interpolations with Several Other Solutions

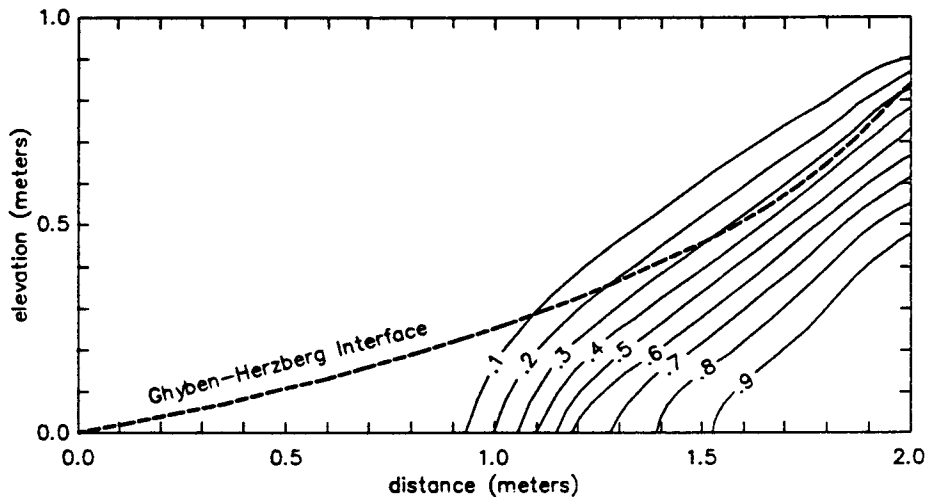


Figure 4. The Complete Set of Isochlors at the Elapsed Time of 300 Minutes; Resulted From the Use of Mixed Interpolations

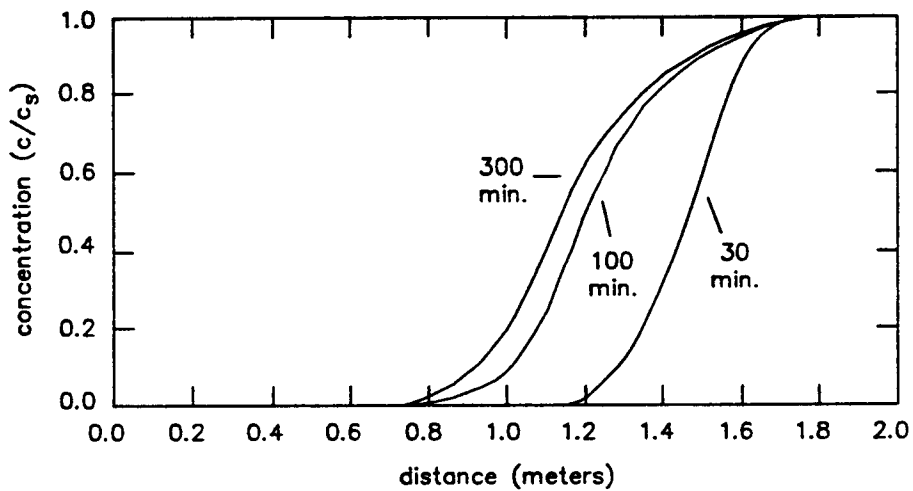


Figure 5. The Transient Variation of Solute-Concentration, Distribution Along the Bottom of the Aquifer; Resulted From the Use of Mixed Interpolations

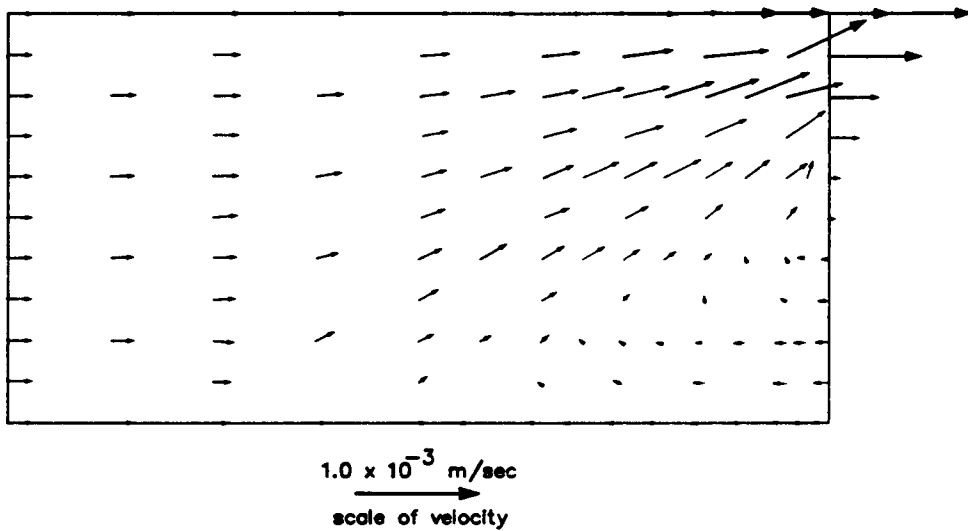


Figure 6. The Calculated Velocity Field for the Elapsed Time of 300 Minutes; Resulted From the Use of Mixed Interpolations

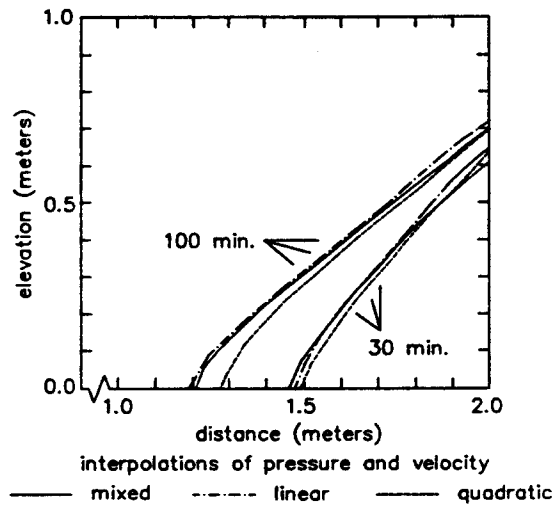


Figure 7. The Comparison of Transient Solutions Obtained From the Use of Different Interpolation Schemes