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Multiphase approach to the numerical solution of a sharp interface saltwater intrusion problem

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Abstract. A sharp interface numerical model is developed to simulate saltwater intrusion in multilayered coastal aquifer systems. The model takes into account the flow dynamics of salt water and fresh water assuming a sharp interface between the two liquids. In contrast to previous two-fluid flow models which were formulated using the hydraulic heads of fresh water and salt water as the dependent variables, the present model employs a mixed formulation having one fluid potential and a pseudosaturation as the dual dependent variables. Conversion of the usual sharp interface flow equations for each aquifer to an equivalent set of two-phase flow equations leads to the definitions of pseudosaturation, capillary pressure, and constitutive relations. The desired governing equations are then obtained by connecting neighboring aquifers via vertical leakage. The proposed formulation is based on a Galerkin finite element discretization. The numerical solution incorporates upstream weighting and nonlinear algorithms with several enhanced features, including rigorous treatment of aquitard leakage and well conditions, and a robust Newton-Raphson procedure with automatic time stepping. The present sharp interface numerical model is verified using three test problems involving unconfined, confined, and multilayered aquifer systems and consideration of steady state and transient flow situations. Comparisons of numerical and analytical solutions indicate that the numerical schemes are efficient and accurate in tracking the location, lateral movement, and upconing of the freshwater-saltwater interface.

Introduction

In coastal aquifers, saltwater intrusion may cause serious consequences in terms of both environmental and economic impacts. The capability to predict the dynamics of saltwater and freshwater is essential in managing water resources in coastal areas. When the two liquids are in contact, they are subject to opposing hydrodynamic mechanisms. Owing to its greater density, saltwater tends to underlie freshwater. At the same time, hydrodynamic dispersion counteracts gravity by providing the tendency to mix the two liquids. The combined effect of these mechanisms gives rise to a transition zone with variable solute concentration. Simulation of the transition zone separating freshwater and saltwater requires simultaneous solution of the governing equations of fluid flow and solute transport. Such an approach leads to density-dependent transport models that are limited in their field application by computational constraints.

An alternative approach for saltwater intrusion study is to model the immiscible flow of fresh water and salt water based on the well-known assumption of an abrupt transition zone or a sharp interface [*Reilly and Goodman*, 1985]. This type of approach facilitates regional-scale studies of coastal areas. Although it does not provide information about the nature of the transition zone, the sharp interface simulator captures the regional flow dynamics and predicts the response of the freshwater/saltwater interface to applied stresses.

The simplest sharp interface formulation is obtained when a single aquifer is considered and saltwater is regarded as static. The flow system is described using only the freshwater equation. The key modeling assumption is known as the Ghyben-Herzberg approximation [*Bear*, 1979]. For problems with regular domains and simple boundary conditions, analytical solutions have been derived [e.g., *Bear and Dagan*, 1964; *Fetter*, 1972; *Strack*, 1976]. For more complicated problems, numerical simulations have been used [*Shamir and Dagan*, 1971; *Ayers and Vacher*, 1983; *Taigbenu et al.*, 1984; *Wirojanagud and Charbeneau*, 1985].

When the dynamics of saltwater becomes important, both the freshwater and saltwater flow equations need to be handled simultaneously. Based on the coupled flow formulation, considerable research has been conducted to investigate saltwater intrusion in single-layer aquifers. In view of the difficulty in developing analytical solutions, most studies relied on numerical methods [*Pinder and Page*, 1977; *Sa da Costa and Wilson*, 1979; *Mercer et al.*, 1980; *Wilson and Sa da Costa*, 1982; *Polo and Ramis*, 1983; *Inouchi et al.*, 1985; *Rivera et al.*, 1990].

For saltwater intrusion in multilayered systems, few modeling studies have been reported, and these are mostly limited extensions of single-layer models [*Mualem and Bear*, 1974; *Sa da Costa and Wilson*, 1979; *Bear and Kapuler*, 1981]. To the best of our knowledge, *Essaid* [1987] was the first to develop a general purpose quasi-three-dimensional, sharp interface model to simulate saltwater intrusion in multiple-aquifer systems. In her work, the block centered finite difference method was used to discretize the coupled saltwater and freshwater flow equations. The block strongly implicit procedure (BSIP)

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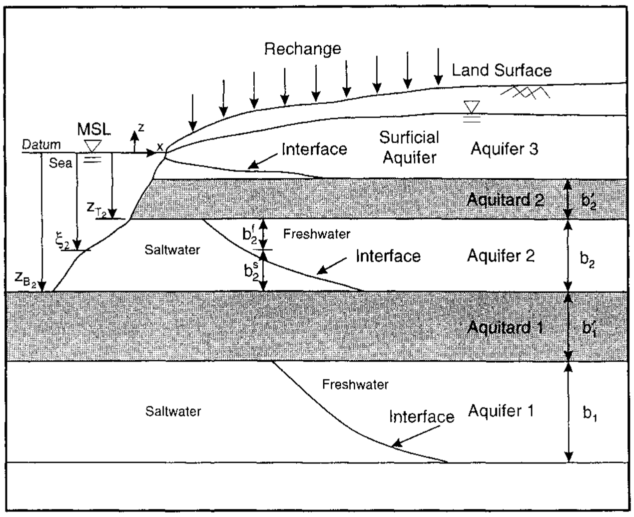

Figure 1. Saltwater intrusion in a multilayered aquifer system.

with Picard iterations was used to solve the matrix equation. To account for the interactions between adjacent aquifers, Darcy's law for density-dependent flux was also used to compute vertical leakage through aquitards. However, this led to leakage schemes that were inconsistent with the key sharp interface (immiscible fluids) modeling assumption. Despite some improvements that may be needed in the formulation, Essaids's model has been a step forward in improving the numerical method for simulating saltwater intrusion in complex aquifer systems.

In this paper, several enhancements are made to the numerical formulation and solution procedures of the sharp interface modeling approach for multilayered aquifer systems. These enhancements include better choice of the dependent variables to yield a more robust mass conservative numerical approximation, less restrictive vertical leakage calculation, rigorous treatment of well conditions, full Newton-Raphson treatment of nonlinearities, and the use of an efficient block Orthomin matrix solver. The numerical schemes are verified using three test problems, including unconfined, confined, and multilayered aquifer and steady state and transient flow situations. Excellent agreement has been obtained for all cases when comparing the model predictions with analytical and other numerical solutions. The test results indicate that the proposed computational algorithms are accurate and efficient in predicting the locations, lateral movement, and upconing of the freshwater-saltwater interface.

Mathematical Development

Governing Equations

Consider a general situation involving a layered coastal aquifer-aquitard system containing freshwater and saltwater domains within each aquifer (Figure 1). It is assumed that the two liquids are separated by a relatively thin transition zone that may be approximated by an abrupt change referred to as the sharp interface. The fresh water forms a pillow (or lens) that is variable in thickness and underlain by the slightly denser salt water. It is also assumed that areal flow of both liquids occurs in each aquifer and vertical leakage without storage occurs in each aquitard. Under these assumptions, the governing equations can be derived by vertical integration of the three-dimensional mass balance equations [*Huyakorn and Pinder*, 1983, pp. 101–109]. For aquifer unit m, which is overlain and underlain by aquitard units m and $m + 1$, respectively, the required equations may be written in the form [*Sa da Costa and Wilson*, 1979, p. 50]

$$\frac{\partial}{\partial x_i}\left(K^f_{ijm} b^f_m \frac{\partial h^f_m}{\partial x_j}\right) + \alpha^f_T \lambda'^f_{m+1}(h^f_{m+1} - h^f_m) + \alpha^f_B \lambda'^f_m (h^f_{m-1} - h^f_m)$$
$$= b^f_m S^f_{sm} \frac{\partial h^f_m}{\partial t} - \theta \frac{\partial \xi_m}{\partial t} - Q^f_m \qquad i, j = 1, 2 \tag{1}$$

$$\frac{\partial}{\partial x_i}\left(K^s_{ijm} b^s_m \frac{\partial h^s_m}{\partial x_j}\right) + \alpha^s_T \lambda'^s_{m+1}(h^s_{m+1} - h^s_m) + \alpha^s_B \lambda'^s_m (h^s_{m-1} - h^s_m)$$
$$= b^s_m S^s_{sm} \frac{\partial h^s_m}{\partial t} + \theta \frac{\partial \xi_m}{\partial t} - Q^s_m \qquad i, j = 1, 2 \tag{2}$$

where superscripts f and s refer to fresh water and salt water, respectively; the primes refer to aquitards; h is the hydraulic head, which is vertically averaged for each aquifer; b^f_m and b^s_m are thicknesses of the freshwater and saltwater zones in aquifer unit m; K^f_{ijm} and K^s_{ijm} are hydraulic conductivities with respect to fresh water and salt water; λ'^l_m $(l = f, s)$ are the leakances of aquitard unit m $(\lambda'^l_m = K'^l_m/b'_m)$; α^l_T and α^l_B $(l = f, s)$ are dimensionless factors set equal to 1 or 0 to indicate the presence or absence of the top and bottom leakages for the aquifer unit; S^f_{sm} and S^s_{sm} are aquifer specific storage coefficients in the freshwater and saltwater zones; θ is the effective porosity; ξ_m is the height of the saltwater-freshwater interface above the datum; and Q^f_m and Q^s_m are volumetric fluxes of freshwater and saltwater due to pumping (or recharge). Note that h^l_{m+1} $(l = f, s)$ corresponds to the heads at the base of the overlying aquitard, and h^l_{m-1} $(l = f, s)$ corresponds to the heads at the top of the underlying aquitard. For the sake of convenience, the datum is placed at mean sea level (msl).

The thicknesses of the freshwater and saltwater zones in aquifer unit m are defined as

$$b^f_m = Z_{Tm} - \xi_m \tag{3}$$

$$b^s_m = \xi_m - Z_{Bm} \tag{4}$$

where Z_{Bm} and Z_{Tm} are the elevations of the base and top of the aquifer, respectively.

The interface position is determined from [*Bear*, 1979]

$$\xi_m = \frac{1}{\varepsilon}\left[(\rho_s/\rho_f)h^s_m - h^f_m\right] \tag{5}$$

where ρ_f and ρ_s are the freshwater and saltwater densities, respectively, and ε is the density difference ratio defined as

$$\varepsilon = (\rho_s - \rho_f)/\rho_f \tag{6}$$

Conversion of Sharp Interface to Two-Phase Flow Equations

If one regards fresh water and salt water as two distinct fluid phases (wetting (w) and nonwetting (n), where w and n correspond to the f (fresh water) and s (salt water) zones of aquifer m, respectively), (1) and (2) can be converted to the conventional two-phase flow equations commonly used in petroleum reservoir engineering. The converted equations may be written in the form

$$\frac{\partial}{\partial x_i}\left(k_{ij}\tau_w \frac{\partial \Phi_w}{\partial x_j}\right) = b\rho_w\left(\beta_{Tw}\frac{\partial \Phi_w}{\partial t} + \theta \frac{\partial S_w}{\partial t}\right) - \dot{M}_w \quad (7)$$

$$\frac{\partial}{\partial x_i}\left(k_{ij}\tau_n \frac{\partial \Phi_n}{\partial x_j}\right) = b\rho_n\left(\beta_{Tn}\frac{\partial \Phi_n}{\partial t} + \theta \frac{\partial S_n}{\partial t}\right) - \dot{M}_n \quad (8)$$

where b is the total liquid-saturated thickness of the aquifer, k_{ij} is the intrinsic permeability tensor, τ_l and Φ_l ($l = w, n$) are vertically integrated mobilities and vertically averaged potentials ($\Phi_l = \rho_l g h^l_m$), respectively, β_{Tl} ($l = w, n$) are fluid storage factors, S_l ($l = w, n$) are phase saturations, and $\dot{M}_l$ ($l = w, n$) are net fluid mass fluxes that include pumping, recharge, and aquitard leakage.

The parameters and variables in (7) and (8) are defined as follows:

$$k_{ij} = \mu_l K^l_{mij}/\rho_l g \qquad l = w, n \quad (9)$$

$$\tau_l = b\rho_l k_{rl}/\mu_l \qquad l = w, n \quad (10)$$

$$b = Z_{Tm} - Z_{Bm} \quad (11)$$

$$k_{rw} = S_w = b^f_m/b \quad (12a)$$

$$k_{rn} = S_n = b^s_m/b \quad (12b)$$

$$S_w = (Z_{Tm} - \xi_m)/b \quad (13a)$$

$$S_n = (\xi_m - Z_{Bm})/b \quad (13b)$$

$$\Phi_w = \rho_f g h^f_m \quad (14a)$$

$$\Phi_n = \rho_s g h^s_m \quad (14b)$$

$$\beta_{Tw} = S_w S^f_{sm}/\rho_f g = S_w \beta_s \quad (15a)$$

$$\beta_{Tn} = S_n S^s_{sm}/\rho_s g = S_n \beta_s \quad (15b)$$

$$\dot{M}_w = \rho_f[Q^f_m + \alpha^f_T \lambda'^f_{m+1}(h^f_{m+1} - h^f_m) + \alpha^f_B \lambda'^f_m(h^f_{m-1} - h^f_m)] \quad (16a)$$

$$\dot{M}_n = \rho_s[Q^s_m + \alpha^s_T \lambda'^s_{m+1}(h^s_{m+1} - h^s_m) + \alpha^s_B \lambda'^s_m(h^s_{m-1} - h^s_m)] \quad (16b)$$

where g is the gravitational acceleration and β_s is the formation compressibility. Note that S_w and S_n as defined in (13a) and (13b) are referred to as pseudophase saturations. In physical terms, S_w and S_n correspond to normalized thicknesses of the freshwater lens and the saltwater wedge, respectively. Similarly, the relative permeability functions defined in (12a) and (12b) are also regarded as pseudoconstitutive relations.

For a surficial (unconfined) aquifer, Z_{Tm} needs to be replaced by h^f_m, which represents the elevation of the water table. Additionally, the definition of β_{Tw} for the unconfined unit needs to be modified as follows:

$$\beta_{Tw} = S_w(bS^f_{sm} + S_y)/b\rho_f g \quad (17a)$$

which may be expressed as

$$\beta_{Tw} = S_w S^{*f}_m/b\rho_f g = S_w(\beta_s + S_y/b\rho_f g) \quad (17b)$$

where $\beta_s = S^f_{sm}/\rho_f g = S^s_{sm}/\rho_s g$, S_{ym} is the coefficient of specific yield assumed to be the same as the drainable porosity θ, and the total saturated thickness and storage coefficient of the unconfined aquifer are defined as

$$b = h^f_m - Z_{Bm} = \Phi_w/\rho_f g - Z_{Bm} \quad (18)$$

$$S^{*f}_m = S^f_{sm} b + S_y \quad (19)$$

To obtain the numerical solution, (7) and (8) are supplemented by the linear relative permeability functions of (12a) and (12b) and the following relations:

$$S_w + S_n = 1 \quad (20)$$

$$\Phi_n = \Phi_w + p_{cnw} \quad (21)$$

where p_{cnw} is the pseudocapillary pressure defined as

$$p_{cnw} = (\rho_n - \rho_w) g \xi_m \quad (22a)$$

Note that (22a) is obtained from (5) by using the definitions of fluid potentials. In terms of S_n, (22a) may be rewritten as

$$p_{cnw} = (\rho_n - \rho_w) g (bS_n + Z_{Bm}) \quad (22b)$$

Initial conditions are required for a transient simulation of the saltwater intrusion problem. These are usually specified in terms of initial distributions of the hydraulic heads. Boundary conditions are also required by the numerical model to obtain a unique solution to the problem. Three types of boundary conditions are usually encountered. These are prescribed head, prescribed flux, and head-dependent flux determined by specifying a head in an adjacent aquifer or surface water body, which causes leakage through a semipervious layer.

In the preceding section, we have converted the mathematical problem of sharp interface saltwater intrusion to the equivalent problem of two-phase flow under vertical equilibrium assumptions and with the use of pseudorelative permeability and capillary functions defined by (12a), (12b), and (22b), respectively.

The initial conditions needed for the numerical solution may be expressed as

$$\Phi_w(x_1, x_2, t) = \Phi^0_w(x_1, x_2) \quad (23a)$$

$$\Phi_n(x_1, x_2, t) = \Phi^0_n(x_1, x_2) \quad (23b)$$

where Φ^0_w and Φ^0_n are the initial, freshwater and saltwater, potentials, respectively.

The boundary conditions of the mathematical problem may be posed in a general form as

$$\Phi_l(x_1, x_2, t) = \tilde{\Phi}_l \qquad \text{on} \quad B_1 \quad (24a)$$

$$\rho_l V_{li} n_i = -\tilde{M}_l \qquad \text{on} \quad B_2 \quad (24b)$$

where $\tilde{\Phi}_l$ and $\tilde{M}_l$ are the prescribed values of fluid potential and mass flux on boundary portions B_1 and B_2, respectively, V_{li} is the Darcy velocity of phase l, and n_i is the outward unit normal vector. Note that $\tilde{M}_l$ is considered positive for inward flux and negative for outward flux.

Numerical Schemes: Discretization

The governing equations represented by (7) and (8) are approximated using the Galerkin finite element procedure. Details of the Galerkin formulation can be found in the work by *Huyakorn and Pinder* [1983]. In a general multilayered case, we discretize each aquifer using the same grid pattern in an areal (x-y) plane. We have modified the conventional Galerkin formulation to incorporate lumping of storage terms and an option to use upstream weighting in calculating phase mobilities. Time integration is performed using a fully implicit (backward difference) scheme.

The freshwater potential Φ_w and the nonwetting phase pseudosaturation S_n are chosen as the primary dependent variables. Since Φ_w and S_n are not the same type of variables, the resulting formulation is referred to as a mixed formulation. To derive the Jacobian matrix, (7) and (8) are discretized and rewritten in the following residual form:

$$R_I^w \equiv A_{IJ}^w \Phi_{wJ} + \frac{B_{II}^*}{\Delta t}[\rho_w(\beta_{TwI}\Delta^t\Phi_{wI} + \theta_I \Delta^t S_{wI})] - F_{wI}^{t+\Delta t} = 0 \tag{25}$$

$$R_I^n \equiv A_{IJ}^n \Phi_{nJ} + \frac{B_{II}^*}{\Delta t}[\rho_n(\beta_{TnI}\Delta^t\Phi_{nI} + \theta_I \Delta^t S_{nI})] - F_{nI}^{t+\Delta t} = 0 \tag{26}$$

where for $l = w$ and n,

$$A_{IJ}^l \Phi_{lJ} = \sum_{J\epsilon\eta_l} \tau_{lIJ}^u \gamma_{IJ}(\Phi_{lI} - \Phi_{lJ}),$$

where I and J are nodal indices ranging from 1 to n, with n being the number of nodes in the grid; Δt is the time increment; $F_l^{t+\Delta t}$ ($l = w$ or n) is a flux vector containing terms that account for sinks and sources, vertical leakage, and boundary bluxes; Δ^t is an operator defined as

$$\Delta^t f = f^{t+\Delta t} - f^t \tag{27}$$

η_l is the set of connecting neighboring nodes; τ_{lIJ}^u is the upstream weighted value of the l phase mobility for the discrete flow between nodes I and J; γ_{IJ} is the transmissivity coefficient for the flow between nodes I and J; and B_{II} is a diagonalized sotrage matrix element.

Application of the Newton-Raphson procedure yields the following system of algebraic equations written in terms of the increments of nodal unknowns, $\Delta\Phi_{wJ}$ and ΔS_{nJ}:

$$\frac{\partial R_I^w}{\partial \Phi_{wJ}}\Delta\Phi_{wJ} + \frac{\partial R_I^w}{\partial S_{nJ}}\Delta S_{nJ} = -(R_I^w)^k \tag{28}$$

$$\frac{\partial R_I^n}{\partial \Phi_{wJ}}\Delta\Phi_{wJ} + \frac{\partial R_I^n}{\partial S_{nJ}}\Delta S_{nJ} = -(R_I^n)^k \tag{29}$$

where

$$\Delta\Phi_{wJ} = \Phi_{wJ}^{k+1} - \Phi_{wJ}^k \tag{30}$$

$$\Delta S_{nJ} = S_{nJ}^{k+1} - S_{nJ}^k \tag{31}$$

and k and $k + 1$ denote previous and current iteration levels, respectively.

With the combined use of the mixed formulation, upstream weighting and full Newton-Raphson procedure, the resulting global matrix system is always mass conservative, positive definite, and suitable for efficient solution by a block matrix iterative technique. Note that the present numerical model does not necessitate an artificial creation of small positive value of saltwater transmissivity in the area where only fresh water exists, and vice versa. Such a procedure was used to improve the matrix condition and avoid numerical difficulties encountered in the previous formulations [*Sa da Costa and Wilson*, 1979, p. 99; *Essaid*, 1990b, p. 50].

Treatment of Boundary Conditions

Boundary conditions associated with the two-phase flow equations describing the sharp interface saltwater intrusion problem can be specified in terms of known (or prescribed) nodal values of fluid potentials (Φ_w and Φ_n) and fluid mass fluxes. These values can readily be converted from the prescribed values of hydraulic heads (h^f and h^s) and volumetric fluid fluxes (Q^f and Q^s).

The prescribed flux boundary conditions are treated simply by adding the specified nodal flux values to the right-hand side of the corresponding nodal equations. If the fluxes are head dependent, then their partial derivatives with respect to the primary variables need to be evaluated and incorporated into the Jacobian matrix.

The prescribed first-type conditions of $\Phi_{lI} = \bar{\Phi}_l$ ($l = w, n$) are incorporated into the matrix system by considering a no-flow condition at node I and then using a source/sink term to inject or produce the correct amount of fluids so that Φ_{lI} approaches the prescribed value $\bar{\Phi}_l$ [*Forsyth*, 1988].

Coastal Boundary Conditions

The boundary conditions at the coastal face of the aquifer system merit special consideration. The boundary conditions of the saltwater flow equation are simply the prescribed saltwater head conditions given by

$$\Phi_{nc} = \rho_s g h_{sc} = \rho_s g z_{\mathrm{msl}} \tag{32}$$

where h_{sc} is the saltwater piezometric head at the coastal face and z_{msl} is the elevation of the mean sea level above the datum.

Since the mean sea level is taken as the datum, (32) becomes

$$\Phi_{nc} = 0 \tag{33}$$

The coastal boundary conditions of the freshwater flow equation may be prescribed by one of two ways. For the sake of convenience, we consider a case of one leaky aquifer overlain by an aquitard. In the first approach the tip of the interface is assumed to be known and corresponding to the top of the aquifer. The freshwater head at the coast, h_{fc}, is then prescribed using (5), which becomes

$$h_{fc} = \frac{\rho_s}{\rho_f} z_{\mathrm{msl}} - \varepsilon\xi_T \tag{34}$$

where ξ_T is the elevation of the tip of the interface. Since the mean sea level is the datum and $\xi_T = z_T$, (34) reduces to

$$\bar{\Phi}_{wc} = \rho_f g h_{fc} = (\rho_s - \rho_f) g d_T \tag{35}$$

where d_T is the depth to the tip of the interface.

In the second approach, it is assumed that the freshwater discharges to the sea and the position of the interface at the coastal face are unknown. The fresh water flows to the sea through a finite opening along the coastline. The discharge of fresh water per unit length of the coastline is determined using the analytical expression derived by *Bear and Dagan* [1964]:

$$Q_{fc} = \rho_f K^f \varepsilon b^f \tag{36}$$

where b^f is the thickness of the freshwater zone at the coast.

In terms of the freshwater potential Φ_{wc} and the d_T, (36) becomes

$$\Phi_{fc} = K_f \rho_f (\Phi_w/\rho_f g - \varepsilon d_T) \tag{37}$$

It should be noted that the head-dependent freshwater flux boundary conditions are implemented with the constraint of $h_f \geq \varepsilon d_T$ to ensure that the fresh water always discharge from the aquifer system to the sea. Thus if the computed h_f is less than εd_T, then Q_f is simply set to zero (i.e., no-flow condition for fresh water).

Treatment of Vertical Leakage

In this section the algorithm for calculating vertical leakage through a leaky aquitard is presented. The present algorithm differs from the previous algorithms presented by *Essaid* [1990a, b] in both how the leakage is computed and how the leakage is distributed.

Our scheme computes the vertical leakage between the same type of liquid and does not allow mixing of different liquids. This approach is coherent with the assumption of a sharp interface, i.e., instantaneous vertical equilibrium of the immiscible fresh water and salt water.

The vertical leakage terms of the freshwater and saltwater flow equations for aquifer unit m may be expressed in a general form as

$$\Gamma_{wm} = \frac{\rho_w}{\mu_w}\left[\alpha_T^f(k'/b')_{m+1}(\Phi_{wm+1} - \Phi_{wm}) + \alpha_B^f(k'/b')_m(\Phi_{wm-1} - \Phi_{wm})\right] \tag{38a}$$

$$\Gamma_{nm} = \frac{\rho_n}{\mu_n}\left[\alpha_T^s(k'/b')_{m+1}(\Phi_{nm+1} - \Phi_{nm}) + \alpha_B^s(k'/b')_m(\Phi_{nm-1} - \Phi_{nm})\right] \tag{38b}$$

where Γ_{wm} and Γ_{nm} are the freshwater and saltwater leakage terms, k'_{m+1} and k'_m are the intrinsic permeabilities of the overlying and underlying aquitards, respectively, and the remaining symbols are as defined previously.

The values of Γ_{wm} and Γ_{nm} depend on the values of the dimensionless leakage parameters: α_B^f, α_T^f, α_B^s, and α_T^s. These parameters are determined using a scheme that identifies the leakage liquids to be of the same types as those at the upstream (or higher potential) points. Furthermore, no mixing of different liquid types is allowed. Thus parameters α_B^l and α_T^l ($l = f, s$) take on the integer value of either 1 or 0, depending on the leaking aquifer conditions.

The freshwater or saltwater leakage between two hydraulically connected aquifers is normally allowed, except for the following cases: (1) fresh water from a particular aquifer unit (referred to as a source unit with a greater fluid potential) cannot leak into a lower aquifer (unit) when the fresh water in the source unit is underlain by salt water; (2) salt water from a source aquifer unit cannot leak into an upper unit when the salt water in the source unit is overlain by fresh water; and (3) the source aquifer does not have the source liquid to discharge (i.e., the upstream liquid mobility is zero). The first and second conditions make certain that the vertical equilibrium is preserved within an aquifer by preventing the lighter liquid from flowing downward through the heavier liquid to reach the underlying leaky aquifer, and the heavier liquid flowing upward through the lighter liquid. The third condition is simply a physical constraint. The three conditions described can be expressed mathematically as follows:

$$\alpha_T^s = 1 \tag{39a}$$

unless $\Phi_{nm} > \Phi_{nm+1}$ and $S_{nm} < 1.0$,

$$\alpha_T^f = 1 \tag{39b}$$

unless $\Phi_{wm} < \Phi_{wm+1}$ and $S_{nm+1} > 0.0$,

$$\alpha_B^s = 1 \tag{39c}$$

unless $\Phi_{nm} < \Phi_{nm-1}$ and $S_{nm-1} < 1.0$,

$$\alpha_B^f = 1 \tag{39d}$$

unless $\Phi_{wm} > \Phi_{wm-1}$ and $S_{nm} > 0.0$,

$$\alpha_T^s = 1 \tag{39e}$$

unless $\Phi_{nm+1} > \Phi_{nm}$ and $\tau_{nm+1} = 0.0$, and

$$\alpha_B^f = 1 \tag{39f}$$

unless $\Phi_{wm-1} > \Phi_{wm}$ and $\tau_{wm-1} = 0.0$.

To incorporate the leakage effect into the freshwater and saltwater flow equations for node I, one needs to obtain the integrated leakage fluxes. These fluxes, denoted by F'_{wmI} and F'_{smI}, are given by

$$F'_{wmI} = \Gamma_{wmI}A_I \tag{40a}$$

$$F'_{nmI} = \Gamma_{nmI}A_I \tag{40b}$$

where A_I is the effective flow area of the node.

Treatment of Pumping Wells

Pumping wells may need to be accounted for in the simulation of the saltwater intrusion problem. We consider a common situation involving withdrawal wells operating under prescribed total production rates. Treatment procedures developed for withdrawal wells can be readily adapted to the corresponding cases of injection wells. We provide a rigorous fully implicit scheme for incorporating the well conditions. This scheme regards the well as a cylindrical source of finite radius and does not rely on the simplifying assumptions for nodal flux calculation. The scheme allows simulation of the local well hydraulic effects on the aquifer system via coupling of analytical and numerical solutions. A well bore of effective radius r_w is considered. For each aquifer the screened section is represented by a single node. The total production rate as contributed by the well nodes is given by

$$Q^T = \sum_{I=1}^{n_s} Q_I^T \tag{41}$$

where Q_I^T is the total fluid flux at node I and n_s is the number of nodes on the well boundary. The total nodal flux Q_I^T is the sum of contributions from fresh water and salt water. Thus, Q_I^T may be expressed as

$$Q_I^T = \sum_l Q_I^l \qquad l = w, n \tag{42}$$

within the control grid-block volume surrounding node I, the flow of each phase is assumed to be in a quasi-steady state and the averaged fluid potential is Φ_{lI}. To facilitate an analytical solution of the local well flow problem, we introduce a concentric circle of radius r_e. The analytical domain is thus bounded by $r_w \le r \le r_e$. Formulas for calculating r_e can be found in several references [*Peaceman*, 1983; *Pritchett and Garg*, 1980; *Abou-Kassem and Aziz*, 1985]. At the well boundary ($r = r_w$), $\Phi_l(r_w) = \Phi_B$, where Φ_B is the averaged potential in the well bore. Using the radial flow analytical solution given by *Dake* [1978, p. 146], Q_{lI} may be expressed as

$$Q_I^l = G_{BI}\tau_{lI}(\Phi_{lI} - \Phi_B) \tag{43a}$$

where G_{BI} is the well bore index for node I and is defined as

$$G_{BI} = \frac{2\pi k \Delta Z_I}{ln(r_e/r_w) + S_F - f} \tag{43b}$$

where f is a constant set equal to 0.75 for transient flow and 0.5 for a steady flow solution, ΔZ_I is the thickness of the control volume surrounding node I, and S_F is a skin factor of the well (S_F is usually set equal to 0). Substituting (43a), (43b), and (42) into (41), Φ_B can be evaluated as

$$\Phi_B = \left(-Q^T + \sum_{I=1}^{n_s} \sum_{l} G_{BI}\tau_{lI}\Phi_{lI}\right) \bigg/ \left(\sum_{I=1}^{n_s} \sum_{l} G_{BI}\tau_{lI}\right) \tag{43c}$$

A fully implicit treatment of the production term of the nodal equation for fluid phase l is obtained by evaluating ΔQ_I^l using the Newton-Raphson expansion. If Φ_w and S_n are the primary variables, then

$$\Delta Q_I^l = \frac{\partial Q_I^l}{\partial \Phi_{wI}} \Delta\Phi_{wI} + \frac{\partial Q_I^l}{\partial S_{nI}} \Delta S_{nI} + \frac{\partial Q_I^l}{\partial \Phi_B} \Delta\Phi_B \tag{44}$$

The unknown $\Delta\Phi_B$ can be eliminated from (44) using (41) and (42) to obtain

$$\Delta Q^T = 0 = \sum_{I=1}^{n_s} \sum_{l} \Delta Q_I^l \tag{45}$$

which upon combining with (44) gives

$$\Delta\Phi_B = \left[-\sum_{I=1}^{n_s} \sum_{l} \left(\frac{\partial Q_I^l}{\partial \Phi_{wI}} \Delta\Phi_{wI} + \frac{\partial Q_I^l}{\partial S_{nI}} \Delta S_{nI}\right)\right] \bigg/ \left(\sum_{I=1}^{n_s} \sum_{l} \frac{\partial Q_I^l}{\partial \Phi_B}\right) \tag{46}$$

The gradients of Q_I^l may be directly evaluated from (43c) as follows

$$\frac{\partial Q_I^l}{\partial \Phi_{wI}} = G_{BI}(\Phi_{lI} - \Phi_B) \frac{\partial \tau_{lI}}{\partial \Phi_{wI}} + G_{BI}\tau_{lI} \frac{\partial \Phi_{lI}}{\partial \Phi_{wI}} \tag{47a}$$

$$\frac{\partial Q_I^l}{\partial S_{nI}} = G_{BI}(\Phi_{lI} - \Phi_B) \frac{\partial \tau_{lI}}{\partial S_{nI}} + G_{BI}\tau_{lI} \frac{\partial \tau_{lI}}{\partial S_{nI}} \tag{47b}$$

$$\frac{\partial Q_I^l}{\partial \Phi_B} = -G_{BI}\tau_{lI} \tag{47c}$$

In summary, the treatment of the well boundary conditions at node I involves the following calculation for each iteration (k).

1. Evaluation of Q_I^l, using (43a) and (43b) and the nodal values from the previous iteration, and addition of Q_I^l to the residual.
2. Evaluation of ΔQ_I^l using (44), (46), and (47a)–(47c).
3. Incorporation of the terms resulting from the Q_I^l evaluation into the Jacobian matrix, and solution of the resulting matrix equation.
4. Evaluation of $\Delta\Phi_B$ using (46).

Nonlinear Iteration and Time Stepping

During each iteration, the linearized system of algebraic equations is solved for the nodal unknowns using an iterative matrix solver based on an incomplete factorization with Orthomin acceleration [*Behie and Forsyth*, 1984]. The nodal values of the primary variables are updated for the next iteration. If necessary, time-step adjustments are made to handle a convergence problem and obtain an efficient transient simulation.

Updating of the nodal values of the unknown variables is performed using an underrelaxation factor determined automatically. The factor is computed based upon the maximum convergence errors for the entire mesh. The following relaxation formula is used to obtain improved estimates of the nodal unknowns:

$$x_I^{r+1} = x_I^r + \Omega^{r+1}\Delta x_I^{r+1} \tag{48}$$

where x_I denotes the nodal unknown variables (Φ_{wI}, S_{nI}), $r + 1$ and r denote current and previous iterations, respectively, and Ω^{r+1} is a relaxation factor for the current iterate.

The value of Ω^{r+1} is determined from

$$\Omega^{r+1} = \max\left[\min\left(\frac{DSNORM}{|e_s^{r+1}|}, 1\right), 0.1\right] \tag{49}$$

where DSNORM is the relaxation norm of saturation and

$$|e_s^{r+1}| = \max_{l,I} |\Delta S_{lI}| \qquad l = w, n \tag{50}$$

with S_l denoting saturation of phase l.

Computational time steps for the transient flow simulation are determined using the following procedure.

1. Start the numerical solution for the first time step with a specified value of Δt_1. Perform the nonlinear Newton-Raphson iterations. If satisfactory convergence is obtained, then determine the subsequent computational time steps using the following algorithm:

$$\Delta t_{k+1} = \min(\tau\Delta t_k, \Delta t_{\max}) \tag{51}$$

where $\Delta t_{\max}$ is the maximum allowable time step size prescribed a priori and τ is the time step multiplier, which is given by

$$\tau = \max\left[\min\left(\frac{\Delta S_{\text{desired}}}{\sum |\Delta' S_l|_{\max}}, 5\right), 10^{-4}\right] \tag{52}$$

where

$$|\Delta' S_l|_{\max} = \max_I |S_{lI}^{k+1} - S_{lI}^k| \tag{53}$$

and $\Delta S_{\text{desired}}$ is the desired incremental changes in pressure and saturation values over the time step.

2. If convergence difficulty is encountered (i.e., solution fails to converge within the allowable maximum number of nonlinear iteration), reduce the computational time step size according to the following scheme:

$$\Delta t_k = \Delta t_k / TDIV \tag{54}$$

where TDIV is the time-step divider.

3. If necessary, adjust the computational time step Δt_k to obtain the t_{k+1} value that coincides with a target time value at which simulation output is required.

Interface Tip and Toe Tracking

In simulating saltwater intrusion using the sharp interface modeling approach, it is often desirable to locate the positions of the interface tip and toe that correspond to the intersections of the interface with the top and bottom of the aquifer, respectively. The tip and toe positions are not necessarily coincidental with the nodal coordinates. However, with the present model, there is no need to resort to any special tip/toe tracking algorithm as used in the previous two models [*Essaid*, 1990b; *Sa da Costa and Wilson*, 1979]. Owing to the use of the mixed formulation, the tip and toe positions at the end of a particular time step may be tracked simply by inputting the computed values of S_n into a standard contouring routine. Since S_n corresponds to the normalized thickness of a saltwater wedge, it is sufficiently accurate for practical purposes to assign the tip and toe locations as corresponding to contours of $S_n = 0.995$ and $S_n = 0.005$, respectively.

Estimation of Salinity of Pumped Water

An estimate of concentration of salt water withdrawn from a pumping well can be provided by the two-fluid, sharp interface model. At the end of each time step, values of integrated fluxes of fresh water and salt water are determined at the well nodes. For node I these flux values correspond to Q_I^f and Q_I^s, respectively (note that $Q_I^f \equiv Q_I^w$, and $Q_I^s = Q_I^n$). The average concentration in water withdrawn from the well, $\bar{c}_{\text{well}}$, is given by

$$\bar{c}_{\text{well}} = \sum_{I=1}^{n_s} (Q_I^s c_s + Q_I^f c_f)/Q_{\text{well}}^T \tag{55}$$

where c_s is the maximum concentration in the salt water, c_f is the background concentration in the fresh water, and Q_{well}^T is the total fluid production rate of the well.

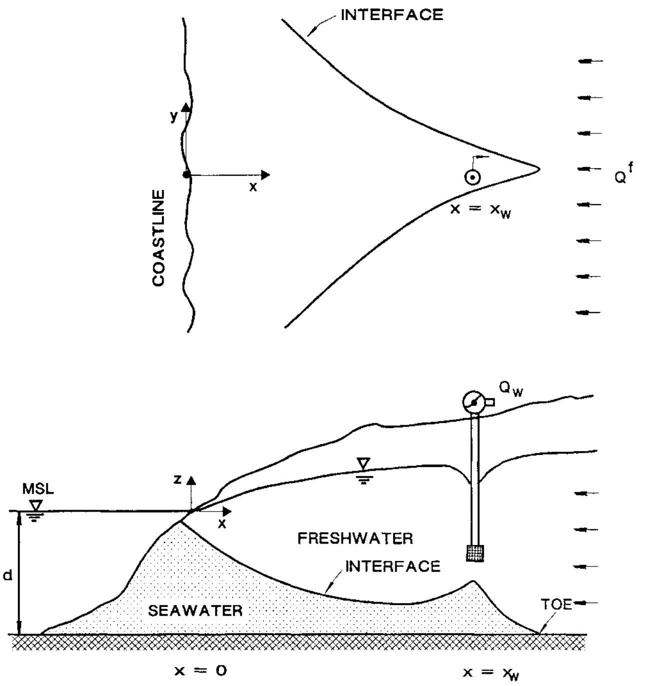

Figure 2. Seawater intrusion and interface upconing in an unconfined aquifer.

Verification

To provide verification of the numerical schemes, three examples are presented. The examples concern (1) seawater intrusion in a coastal unconfined aquifer, (2) seawater intrusion in a two-layered aquifer system separated by a leaky aquitard, and (3) interface upconing beneath a pumping well in a confined aquifer. Note that the problems considered are characterized by different hydrogeologic settings and steady state and transient flow situations. For the first two examples, numerical simulation results are compared with analytical solutions. For the third example, a comparison is made between numerical solutions obtained from the present sharp interface model and a more rigorous multiphase numerical model. In all cases, freshwater and saltwater densities are taken as 1000 kg/m^3 and 1025 kg/m^3, respectively.

Seawater Intrusion in a Coastal Unconfined Aquifer

This example concerns seawater intrusion in an areal plane of an unconfined aquifer with a pumping well near the coastline. The well withdraws fresh water only, causing upconing of underlying salt water. A schematic description of the problem is illustrated in Figure 2. *Strack* [1976] derived a steady state analytical solution using a special potential function. The following parameter values were used in verifying the numerical model:

Freshwater flux Q^f	1 m^2/d (at $x = 1000$ m, $0 \le y \le 2000$ m)
Well pumping rate Q_w	400 m^3/d
Well location (x_w, y_w)	(600 m, 0)
Hydraulic conductivity, K	70 m/d
Depth from msl to aquifer base	20 m

Strack's analytical solution is based on the assumption of an areally semi-infinite aquifer. For the case used to test the numerical solution, a rectangular domain, depicted in Figure 2, was adopted. This test case is identical to that used by *Sa da Costa and Wilson* [1979] to verify their sharp interface, finite element model. We modified Strack's solution by placing an imaginary pumping well at $(x_{iw}, y_{iw}) = (600 \text{ m}, 4000 \text{ m})$ to account for the closed boundary at $y = 2000$ m.

Owing to symmetry about the y axis, only the upper half plane was discretized. A nonuniform rectangular grid consisting of 209 nodes (11 rows by 19 columns) was used. Minimum grid spacings of 5 m, along the x and y axes, were used to accommodate steep hydraulic gradients near the pumping well. Seawater coastal boundary conditions were used at the coastline ($x = 0$). Constant freshwater influx was specified at the inland boundary ($x = 1000$ m). A no-flux condition was used for other boundaries. The numerical results were obtained with and without the use of upstream weighting. Simulated profiles of the steady state interface and water table along the x axis are depicted in Figure 3 together with the analytical solution.

The numerical model required considerably fewer nonlinear iterations when upstream weighting was used. Note, however, that the nonupstream (Galerkin finite element) numerical solution is in good agreement with the analytical solution. The nonupstream interface profile exhibits only slight oscillations. On the other hand, the upstream numerical solution is nonoscillatory but smeared due to the coarseness of the grid. In order to improve the accuracy of the upstream numerical solution, a refined grid consisting of 861 nodes (21 rows by 41 columns) was adopted, and the model was rerun. The result is much improved and in good agreement with the analytical solution.

Seawater Intrusion in a Multilayered System

This example is described schematically in Figure 4a. *Mualem and Bear* [1974] derived a steady state analytical solution for the depicted situation involving a two-layer coastal aquifer system separated by a thin aquitard. Their solution was based on the Dupuit assumption and linearization of the flow

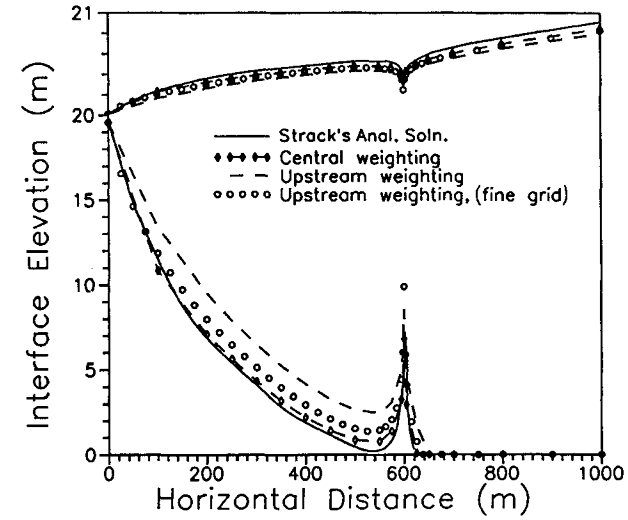

Figure 3. Steady state profiles of the interface and water table simulated for the coastal unconfined aquifer example.

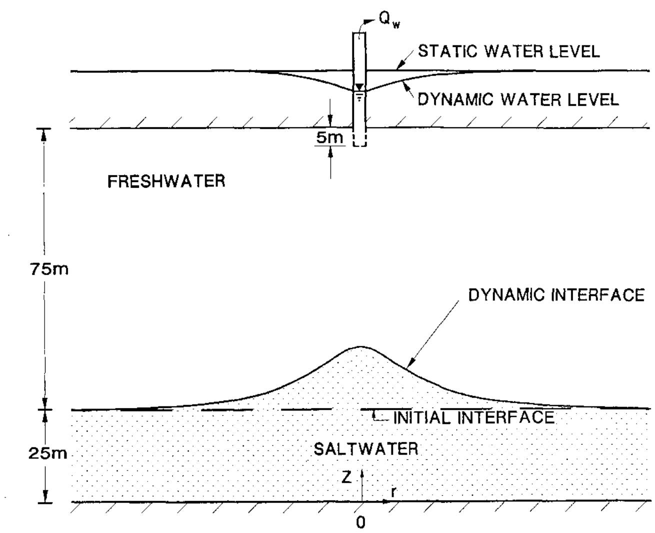

Figure 5. Interface upconing beneath a pumping well.

equation. As given in Figure 4b, the chosen parameter values may be viewed as representing the scales of a sandbox experiment. The freshwater flow Q_f was specified per unit width. For numerical simulation, the aquifer system was represented by a uniform rectangular mesh consisting of 96 nodes (2 rows by 48 columns). Freshwater flux boundary conditions were applied at the inland boundary, and coastal boundary conditions were applied at the seaward boundary. The analytical and numerical solutions are compared in Figure 4b. The numerical results were obtained with upstream weighting. Considering that the analytical solution is approximate due to linearization, agreement between the two solutions is reasonable. The analytical solution was obtained using the interface position at the landward end of the aquitard as a boundary condition. Therefore no analytical solution is available in the region of the aquifer where there is no aquitard.

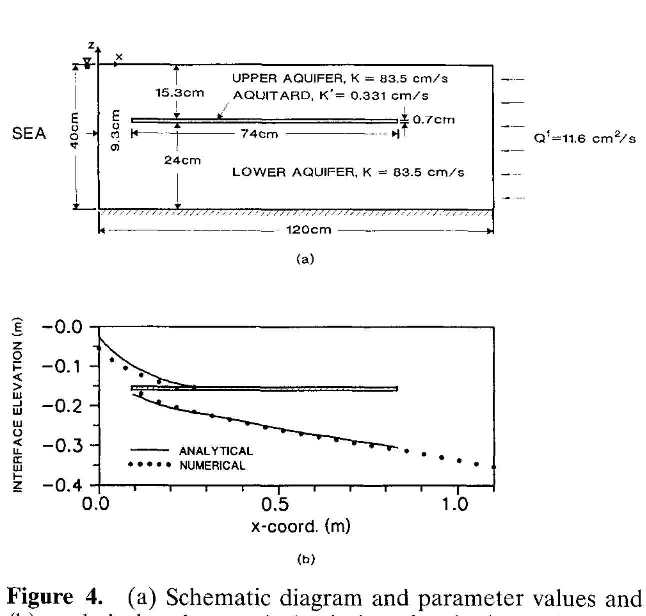

Figure 4. (a) Schematic diagram and parameter values and (b) analytical and numerical solutions for the layered aquifer example.

Transient Interface Upconing Beneath a Pumping Well

Although the previous two examples provide the model verification for saltwater intrusion in single-layer and multilayered aquifer systems, they are limited to steady state conditions. In view of this, we include a third example involving transient interface upconing.

The situation of interest concerns upconing of the freshwater-saltwater interface below a partially penetrating well pumping from a confined aquifer. A schematic description of the problem is shown in Figure 5. Initially, the aquifer is in hydrostatic equilibrium and the underlying interface is horizontal. Groundwater withdrawal from the well causes drawdown of the piezometric surface and upconing of the interface. In this example, we elect to use a rigorous multiphase three-dimensional numerical code MAGNAS [*Huyakorn et al.*, 1994a] to examine the simulation results of the sharp interface saltwater intrusion code (SIMLAS). This is because the sharp interface concept can be treated as a special case of the multiphase model, when the gravity segregation vertical equilibrium (GSVE) condition exists [*Huyakorn et al.*, 1994b]. Furthermore, the saltwater upconing problem considered here is analogous to the water upconing problem in the petroleum literature [*Muskat*, 1982]. In order to ensure the GSVE flow condition, some special procedures were taken in the multiphase simulation, as follows: (1) freshwater and saltwater were regarded as "oil" and "water," respectively, with zero capillary pressure between the two "phases"; (2) the relative permeability for each phase was set equal to the phase saturation; and (3) a high value of vertical anisotropy ratio (k_z/k_x) was assumed.

The aquifer was assumed to be homogeneous, and the parameter values used were as follows:

Horizontal permeability k_x, k_y	1×10^{-12} m^2
Vertical permeability k_z	5×10^{-9} m^2
Porosity ϕ	0.20
Aquifer thickness b	100 m
Pumping rate of well Q_w	50 m^3/d
Distance from the well bottom to the initial interface d	70 m
Well screen length L	5 m
Height of the initial interface above the aquifer base z_0	25 m

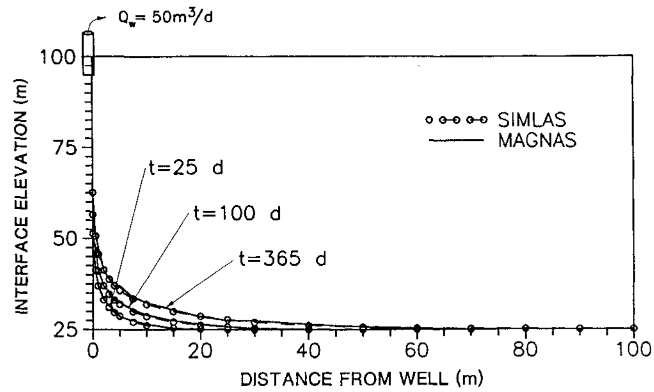

Figure 6. Simulated profiles of the transient interface for the local upconing example at $Q_w = 50$ m^3/d.

For the sharp interface areal model the aquifer domain was assumed to be a square of dimensions 2000 m by 2000 m, with the well at the center. Owing to symmetry, only the first quadrant of the domain was discretized using a nonuniform rectangular grid consisting of 1600 nodes (40 rows by 40 columns). The numerical simulation was performed using upstream weighting and the automatic time-stepping scheme described previously. For the rigorous multiphase solution, the domain was represented by a cylinder of radius 2000 m and thickness 100 m. An axisymmetric (r, z) grid was used, and the discretization in the radial direction was the same as the sharp interface grid, and the vertical dimension was subdivided into 35 rows, with a total of 1400 nodes. Time steps were also generated automatically.

Shown in Figure 6 are simulated profiles of the interface at different time values predicted for a pumping rate of 50 m^3/d. There is excellent agreement in the results obtained from the two models. Figure 6 also indicates that the salt water has not yet broken through, and the long-time solutions from both models confirm that no salt water enters the well under the proposed conditions. If the pumping rate is increased to 100 m^3/d, the exacerbation of saltwater upconing is shown in Figure 7. Again the two numerical solutions are in excellent agreement. However, the salt water enters the well after 10 days because of the higher pumping rate.

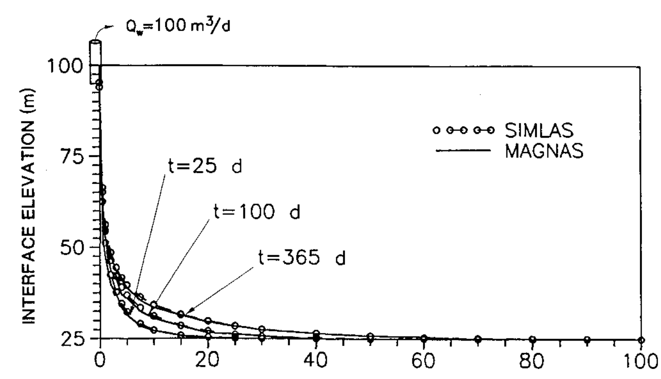

Figure 7. Simulated profiles of the transient interface for the local upconing example at $Q_w = 100$ m^3/d.

Concluding Remarks

A two-phase formulation of saltwater intrusion problems in multilayered coastal aquifers has been developed. The formulation utilizes the freshwater potential and pseudosaturation directly related to the interface elevation as the dual dependent variables. The advantage of such a formulation is twofold. First, the matrix system resulting from the upstream-weighted, finite element or finite difference approximation and the Newton-Raphson linearization is always mass conservative and highly stable. There is no need for an artificial assignment of a small positive value of saltwater or freshwater transmissivity in the area where only one fluid exists. Second, the positions of the toe and tip of the interface can be easily tracked because the interface elevation is directly obtained from the numerical solution.

The proposed numerical schemes have been verified using a series of test problems with different hydrogeologic settings and steady state and transient flow situations. Comparisons of numerical and analytical solutions were made for unconfined, confined, and leaky multilayered systems. The comparison study has shown that our computational algorithms are accurate in tracking the location and lateral movement and upconing of the freshwater-saltwater interface.

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