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原著

다중 다상이론을 이용한 통합적 지하수 모델링: 1. 다차원 유한요소 모형의 개발

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A Comprehensive Groundwater Modeling using Multicomponent Multiphase Theory: 1. Development of a Multidimensional Finite Element Model

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ABSTRACT

An integrated model is presented to describe underground flow and mass transport, using a multicomponent multiphase approach. The comprehensive governing equation is derived considering mass and force balances of chemical species over four phases(water, oil, air, and soil) in a schematic elementary volume. Compact and systemati notations of relevant variables and equations are introduced to facilitate the inclusion of complex migration and transformation processes, and variable spatial dimensions. The resulting nonlinear system is solved by a multidimensional finite element code. The devolped code with dynamic array allocation, is sufficiently flexible to work across a wide spectrum of computers, including an IBM ES 9000/900 vector facility, SP2 cluster machine, Unix workstations and PCs, for one-, two and three-dimensional problems. To reduce the computation time and storage requirements, the system equations are decoupled and solved using a banded global matrix solver, with the vector and parallel processing on the IBM 9000. To avoide the numerical oscillations of the nonlinear problems in the case of convective dominant transport, the techniques of upstream weighting, mass lumping, and elementary-wise parameter evaluation are applied. The instability and convergence criteria of the nonlinear problems are studied for the one-dimensional analogue of FEM and FDM. Modeling capacity is presented in the simulation of three dimensional composite multiphase TCE migration. Comprehesive simulation feature of the code is presented in a companion paper of this issue for the specific groundwater flow and contamination problems.

Key word : integrated groundwater model, multidimensional finite element method, multicomponent multiphase system

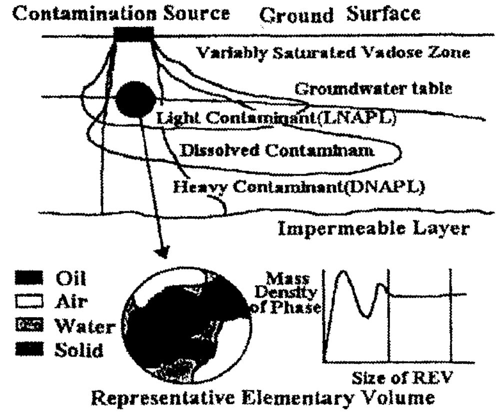
요 약 문

지하의 유체 유동 및 물질 변환을 해석하기 위하여 다중다상이론을 이용한 통합 모형을 개발하였다. 종합적 지배식은 4개의 상내의 화합물들의 물질 및 힘평형 관계를 고려하여 유도되었다. 복합한 이동 및 변환 현상을 설명하고, 공간적 차원을 변동적으로 나타내기 위하여 관계된 모든 변수 및 식들을 함축적이면서 조직적으로 표현하였다. 도출된 비선형시스템은 다차원 유한요소프로그램으로서 해를 구하였다. 본 개발된 프로그램은 역동적으로 메모리 용량을 조절하여 일이삼차원 문제를 PC부터 SP2 슈퍼컴퓨터까지 여러 종류의 기종에서 해석할 수 있다. 계산시간과 저장용량을 줄이기 위하여 시스템식을 분리시키고, 슈퍼컴의 벡터 및 병렬처리를 이용하여 띠행렬의 해를 구하였다. 유속이 우세한 경우의 수치해석상의 불안정한 문제를 해결하기 위하여 상류가중, 질량묶음, 요소별 파라미터 평가법 등을 적용하였다. 일차원 이동문제에 대하여 유한요소법과 유한차분법의 수치해의 안정성 조건을 검토하였다. 구체적인 지하수 유동 및 오염문제에 대한 모델링 예는 본 논문집의 연계 논문에 수록하였다.

주제어 : 통합 지하수모형, 다차원유한요소법, 다중다상이론

1. INTRODUCTION

The derivation of the theory for immiscible flow and mass transformation started with the application of continuos partial differential equations over the discontinuous domain, using the traditional averaging concepts in continuum mechanics(Bear, 1979;Bachmat and Bear, 1986; Hassanizadeh and Gray, 1979a, b) as shown in Fig. 1. To overcome the length scale problem in the volume averaging concept, a hierachic sequence was used(Celia et al., 1993). In this study, a simple schematic control volume in Fig. 2 is constructed to derive mass and force balance equations in a intregrated model.



1. Idealized migration profile and REV.

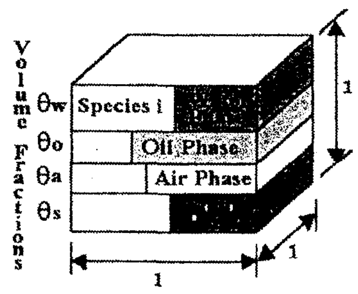


Fig. 2. Schematic conrtol volume.

Lin and Gray(1971) presented one of the earliest studies related to multiphase force balance. They derived a steady state momentum equation for laminar flow in capillary tube, in which head difference, capillary pressure, and surface tension were included. The theoretical equations were verified against experimental tests of capillary tubes. Hassanizadeh and Gray (1979a, 1979b), Allen(1984), and Abriola(1984) have rigorously derived the modified Darcy's velocity from the momentum equation. Kueper and Frind(1988) examined the effects of density, viscosity, surface tension on interfacial immiscible displacements when reviewing immiscible fingering, based upon a force blance of pressure, gravity force, viscous friction, and interfacial surface tension. Gray and Hassanizadeh(1991a, b, 1993) showed the paradox, if the modified Darcy's velocity is used in a variably saturated region, which requires false negative water phase pressure in capillary-saturation relations. To overcome the problem, they developed a multiphase momentum equation including interfacial dynamics based on conservation of mass, momentum, and energy, and the second law of thermodynamics. Application of their technique required experimental data to ascertain the constitutive coefficients. Beckie et al.(1993) presented a mixed formulation of the continuity and momentum euqations for simple saturated groundwater flow, and performed large-scale finite element simulation using a multigrid, accelerated domain decomposition technique. Considering all the studies mentioned above, one can solve the multiphase momentum equation or use the modified Darcy's equation to describe velocity profile in a multicomponent multiphase problem.

A brief review of previous groundwater modeling efforts is presented to provide background and support with respect to:1) finite difference models, 2) finite element models, 3) front tracking models, 4) boundary element models, 5) analytical solutions, and 6) vector and parallel processing.

Kuepper and Frind(1991a) developed a two-dimensional finite difference model to solve the wetting phase pressure and saturation, which eliminated the need to specify small, fictitious saturations of nonwetting fluid phase of the advancing front. The model is verified against an exact analytical solution, and a parallel-plate laboratory experiment involving the infiltration of TCE into a heterogeneous sand pack (Kuepper and Frind, 1988). Kuepper and Frind (1991b) applied the model to a field problem based on the laboratory measurements of capillary-saturation and permeability curves of samples. They asserted that the migration of a nonwetting liquid was extremely sensitive to subtle variations of capillary and fluid physical properties. Sleep and Sykes(1993a) developed a compositional model including several numerical options, ranging from fully implicit with first-order upstream weighting to implicit in pressure, explicit in saturations and concentrations with third-order upsteam weighting. The model was verified to the extent possible with analytical solutions for simplified cases of multiphase flow and contaminant transport. The accuracy and efficiency of the various numerical options in the model were illustrated. Sleep and Sykes(1993b) demonstrated the effect of field scale heterogeneities on the movement of organic compounds. The influnce of infiltrating wetting fronts on gas phase transport of volatile organic compounds was shown to be significant. The long-term fate of a subsurface spill of a three-component dense organic liquid was simulated. Three-dimensional simulation of soil vacuum extraction demonstrated the difficulty in removing dissolved organic compounds from the saturatede zone. Adenekan et al.(1993) developed a compositional simulator for three-dimensional, nonisothermal, multicomponent multiphase transport. The model's distinct features are that it can simulate the transport of sensible and latent heat energy, and that each phase was allowed to completely disappear from, or appear in any region of the domain.

Kim(1989) developed a comprehensive groundwater model to simulate a wide range problems from unsaturated flow to composite multiphase contaminant migration using a multidimensional finite element method. This paper is based in part upon the results of his dissertation. Mendoza and Frind(1990a) used standard Galerkin FEM technique and triangular elements for dense organic vapor transport in the unsaturated zone. Axisymmetric coordinates were used to represent localized residual saturation solvent sources, and the model was compared to three-dimensional laboratory experiment. Mendoza and Frind(1990b) showed that mass transport were highly dependent upon diffusion for compounds with high vapor pressure and molecular weights in coarse sands or gravels media. Wood and Calver(1990) compared distributed mass matrix to lumped one for the solutions of Richards' equation, and found no difference in run times and convergence rate, but significant discharge difference. Celia and Binning(1992) presented a mass conservative numerical solution of water-air phase system based on a modified Picard linearization of the governing equations, coupled with a lumped finite element approximation in space and dynamic time control. Cordes and Kinzibach(1992) used head gradients of adjacent elements to compute discontinuous Darcy velocity fields using the concept of flux-conserving boundaries. Miller and Rabidearu(1993) proposed one-and two-dimensional split-operator method in which the reaction operator of sorption and desorption were separated from the transport operator and solved independently with Petrov-Galerkin method.

Several researchers have investigated front-tracking algorithms, such as the Eulerian-Lagrangian method. Yeh(1990) presented one- and two-dimensional LE(Lagrangian-Eulerian) method with automatic mesh adaptation for the sharp front regions of solute transport equation. Comparison of upstream FEM, LE, LEZOOM, and exact solutions indicated that LE approach was superior to UFE method. Schafer-Perini and Wilson(1991) presented a dynamic front tracking algorithm for two-dimensional groundwater flow to save storage and computational expense. Ryan and Cohen(1991) proposed a one-dimensional front-tracking algorithm to determine the front of the invading NAPL as a function of penetration time based on four dimensionless functional groups in two-phase simulations. Bentley and Pinder(1992) developed several algorithms to overcome the tracking error problems of Eulerian-Lagrangian methods, such as the accuracy of the integration and the particle velocity. They presented a dynamically adjusted second-order Runge-Kutta method, a Crank-Nicholsen method for source terms, and a time step size based on the local velocity. Gottardi and Venutelli(1992) presented a moving finite element method for Richards' equation, in which grid points are moved along with the wetting front. Newman(1993) presented a unified Eulerian-Lagrangian theory for conservative solute transport in a random velocity field where the spatial derivative of velocity vector was a random function of the sources and/or time derivative of head. Connell and Bell(1993) presented a moving node finite element method(MFE) to solve the system of partial differential equation of water and air phase flow for oil shale waste dump. The hydraulic conductivity, moisture retentivity, water vapor-air diffusivity, and intrinsic permeability of air were estimated based upon field measurements.

Stothoff and Pinder(1992) developed a boundary integral formulation for flow of two immiscible, incompressible phases. Boundary integral meshes were placed along contours of phase saturation, and the contours were updated with time, based on phase fluxes. The model was verified against an exact solution, and the solution of finite element simulator for one-dimensional radial two-phase flow. Khanbilvardi et al.(1993) presented two boundary integral methods. The first directly used Green's function. Both techniques simulated unsaturated moisture flow using time dependent fundamental solution of the governing equation, and verified against the exact solution. Cheng and Morohunfola(1993 a, b) developed a boundary element algorithm for one- and two-dimensional, pumping well problems in multilayered leaky aquifer.

To verify the numerical models mentioned above, the best choice is to derive the analytical solutions. Since the 1960's, many analytical solutions have been developed for the infiltration problems, such as the Richards equation: (McWhorter, 1971, 1992; Noblac and Morel-Seytox, 1972; Warrick et al., 1990; Ross, 1990; Srivastava and Yeh, 1991; Warrick et al. 1991; Kirkland et al., 1992; Parkin et al., 1992). However, little improvement has been made for the multiphase flow problems.

All the previously cited numerical techniques can be computationally intensive. Ressearchers have investigated techniques to improve accuracy and reduce computation time. Pelka and Peters(1986) proposed program techniques to fully utilize vector and parallel computers, requiring additional intrinsic vector functions beyond the Fortran 77 standard, and more memory. The barriers to vectorization were: (1) conditional and branch statements, (2) sequential dependencies; (3) nonlinear and indirect indexing; (4) subroutine calls within loops and (5) recursive operations. Dougherty (1991) showed tutorial examples of the random walk, Poisson's equation, and modeled steady state three-dimensional groundwater flow using the parallel processor in a Connection Machine (CM-2). A diagonally preconditioned conjugate gradient (DPCG) solver was applied to practical problem to show the performance of DPCG on the CM-2. Tripathi and Yeh(1993) compared run times of a program on scalar, RISC and vector computers. RISC based scalar computers such as IBM 6000/560 provided the best performance-to-price ratio.

The objectives of this study are: 1) to develop a comprehensive code to solve many different groundwater flow and pollution problems with the proper choice of parameters such as mass fraction and saturation coefficients, 2) to search optimal numerical techniques for handing the very unstable properties of the nonliner partial differential equations, and 3) to reduce the data and parameter requirements of the code.

2. THEORETICAL BACKGROUND

Macroscopic mass balance equation is expressed as follows for nonequilibrium conditions:

$$\frac{\partial C^i_\alpha}{\partial t} + \nabla (C^i_\alpha \vec{V}_\alpha) = \nabla (\mathbf{D}^i_\alpha \nabla C^i_\alpha) + I^i_\alpha + g^i_\alpha \cdots (2.1)$$

where, $\mathbf{D}^i_\alpha (= \mathbf{D}^i_{h,\alpha} + \mathbf{D}^i_{m,\alpha})$ is disperisve coefficient tensor, and I^i_α is the interfacial mass transfer rate for mass exchange by means of dissolution, sorption, volatilization, ion exchange, and diffusion.

The overall migration process of the four phases depends upon the migration process of each phase. Thus, total migration of species i is msummation of equation (2.1) over all phases. To include the effects of volumetric fraction, density, and mass fraction of each phase, equation (2.1) is multiplied by volumetric fraction. The final form of multiphase mass transport equation of species i is expressed as follows:

$$\sum_{\alpha=1}^{4}\left[\frac{\partial(\theta_\alpha \rho_\alpha w^i_\alpha)}{\partial t} + \nabla(\theta_\alpha \rho_\alpha w^i_\alpha \vec{V}_\alpha)\right.$$

$$\left. = \nabla(\theta_\alpha \mathbf{D}_\alpha{}^i \nabla(\rho_\alpha w^i_\alpha)) + \theta_\alpha I^i_\alpha + \theta_\alpha g^i_\alpha\right] \cdot (2.2)$$

where, $\theta_\alpha (= U_\alpha \mid U = \phi S_\alpha)$ = volumetric fraction, $S_\alpha (U_\alpha \mid U_v = U_\alpha (\phi U) = \theta_\alpha \mid \phi)$ = saturation, U_α = volume of the α phase, U = volume of all phases, ϕ = aquifer porosity, $\rho_\alpha (= M_\alpha \mid U_\alpha)$= density of α phase, M_α= mass of the phase, w^i_α (=$M^i_\alpha \mid M_\alpha$) = mass fraction of species, M^i_α = mass of species in the α phase.

Including the interfacial momentum exchange, a macroscopic momentum equation is derived through the extension of the density and pressure of each species to all species in each phase:

$$\sum_{i=1}^{ns}\left[\rho_\alpha w^i_{alph} \frac{D\vec{V}^i_\alpha}{Dt} = -\nabla(P^i_\alpha + \rho_\alpha w^i_\alpha g y)\right.$$

$$\left. + \mu_\alpha \nabla^2 \vec{V}^i_\alpha + \vec{R}_\alpha\right] \cdots\cdots (2.3)$$

where, ns the is total number of species in the α phase, $\vec{R}_\alpha$ is the modefied momentum exchange in the form of an isotropic Stokes' drag force (Allen, 1984), which denotes the resistance to motion of the i component in α fluid phase by a slowly moving or immovable component in soil phase, acting in a direction opposite to the flow of the fluid phase.

It is possible to neglect the inertia term of the momentum equation due to the slow velocity of fluid phase. After neglecting the composite effect of the components in each phase ($\sum \rho_\alpha w^i_\alpha = \rho_\alpha \sum P^i_\alpha = P_\alpha \sum R^i_\alpha = R_\alpha$), and the viscous effects, the velocity of the α phase in a deformable porous media becomes:

$$\vec{V}_\alpha = -\frac{K_\alpha}{\phi_\alpha \mu_\alpha} \nabla (P_\alpha + \rho_\alpha g y) + \vec{V}_s$$

$$= -\mathbf{k}\frac{k_{ra}}{\theta_\alpha \mu_\alpha} (\nabla P_\alpha - \rho_\alpha \vec{g}) + \vec{V}s \cdots\cdots (2.4)$$

where, $\mathbf{k}$ is the intrinsic permeability tensor, $k_{r\alpha}$ is the relative permeability of the α phase, $\vec{g}$ is the downward vector of gravity force.

If there is no change of total stress of overburden load, the compressibility of the porosity by pressure head is defined as $\phi_\beta = (\partial\phi) \mid (\partial h_\beta)$, then solid transport equation is expressed in terms of compressible porosity, phase head, and solid velocity.

$$\sum_{\beta=1}^{3} (\phi_\alpha \frac{\partial h_\beta}{\partial t}) = \nabla (1-\phi)\vec{V}_s \cdots\cdots (2.5)$$

The compressibility ϕ_β is obtained experimentally from the constitutive equation. The fluid pressure h_β is computed from the whole multicomponent multiphase system. The velocity of the solid phase and the time rate change of porosity are computed from equation (2.5). For an elastic soil matrix, the parameter ϕ_β is constant; for a nonelastic soil, it is dependent upon pressure and properties of soil matrix, and the system becomes highly nonlinear. For contaminant migration problems, the elastic deformation assumption is usually accepted. ϕ_β is incorporated into the fluid equation by specific storativity as follows:

$$S_{\alpha\beta} = \phi_\beta + \phi_{\alpha\beta} \cdots\cdots (2.6)$$

where, $\alpha_\beta (= \partial \rho_\alpha) \mid (\rho_\alpha \partial h_\beta)$ is the compressibility of the α phase by the β pressure head, and $S_{\alpha\beta}$ is the specific storativity of the porous matrix and fluid. α_β and ϕ_β always have negative values.

By assuming isothermal conditions and neglecting the density change due to concentration, the storage capacity of the system can be expressed as follows:

$$w^i_\alpha S_\alpha \frac{\partial(\phi\rho_\alpha)}{\partial t} = w^i_\alpha S_\alpha (\rho_\alpha \frac{\alpha\phi}{\partial t} + \phi \frac{\partial \rho_\alpha}{\partial t})$$

$$= \rho_\alpha w^i_\alpha S_\alpha \sum_{\beta=1}^{3} (\frac{\partial\phi}{\partial h_\beta} + \frac{\phi}{\rho_\alpha}\frac{\partial\rho_\alpha}{\partial h_\beta})\frac{\partial h_\beta}{\partial t} = \rho_\alpha w^i_\alpha S_\alpha \sum_{\beta=1}^{3} S_{\alpha\beta} \cdots\cdots (2.7)$$

Separating the solid phase from the time derivative, including the Darcy and solid velocity, and storage capacity of porous media, the integrated transpor equation is expressed as follows:

$$\sum_{\alpha=1}^{3}\left[\sum_{\beta=1}^{3}(\rho_\beta w^i_\beta S_\beta \beta\alpha)\frac{\partial h_\alpha}{\partial t} + \phi\rho_\alpha w^i_\alpha \frac{\partial S_\alpha}{\partial t} + \phi\rho_\alpha S_\alpha \frac{\partial w^i_\alpha}{\partial t}\right]$$

$$+ \frac{\partial(1-\phi)\rho_s w^i_s}{\partial t}$$

$$\sum_{\alpha=1}^{3}\left[\nabla\left[\rho_\alpha w^i_\alpha \mathbf{K}_\alpha\left(\nabla h_\alpha + \frac{\rho_\alpha}{\rho_w} j\right)\right] + \nabla(\phi S_\alpha \mathbf{D}^i_\alpha \nabla(\rho_\alpha w^i_\alpha))\right]$$

$$- \nabla((1-\phi)\rho_s w^i_s \vec{V}_s) + \sum_{\alpha=1}^{4}[\theta_\alpha(I^i_\alpha + g^i_\alpha)] \cdots\cdots (2.8)$$

3. MULTIDIMENSIONAL FINITE ELEMENT MODEL

Applying the integrated element matrices, element-wise parameters, and Green's theorem, the weighted residual form of the governing equation is discretized as follows:

$$\sum_{e=1}^{nel}[\sum_{j=1}^{nn}[\sum_{\alpha=1}^{na}[[EM_{i,j}]\left\{\left(\sum_{\beta=1}^{na}(\rho_\beta w^i_\beta S_{\beta\alpha})_j\right)\frac{\partial h_{\alpha,j}}{\partial t}\right.$$

$$\left. + (\phi\rho_\alpha w^i_\alpha)_j \frac{\partial S_{\alpha,j}}{\partial t} + (\phi\rho_\alpha S_\alpha)_j \frac{\partial w_{\alpha,j}}{\partial t}\right\}$$

$$+ \sum_{id=1}^{nd}\sum_{jd=1}^{nd}[ED_{id,jd,i,j}](\rho_\alpha w^i_\alpha \mathbf{K}_\alpha) h_{\alpha,j} + (\phi S_\alpha \rho_\alpha \mathbf{D}^i_\alpha)_j w^i_{\alpha,j}$$

$$+ [EM_{i,j}]\frac{\partial}{\partial t}((1-\phi)\rho_s w^i_s)_j]]$$

$$= \sum_{\alpha=1}^{na}[\sum_{j=1}^{nn}[-[EV_{i,j}]\left(\rho_\alpha w^i_\alpha \mathbf{K}_\alpha \frac{\rho_\alpha}{\rho_w}\right)_j$$

$$+ [EM_{i,j}](\phi S_\alpha (I^i_\alpha + g^i_\alpha)_I)$$

$$+ \int w_{ib}\rho_\alpha w^i_\alpha \mathbf{K}_\alpha \left(\nabla h_\alpha + \frac{\rho_\alpha}{\rho_w}\vec{j}\right)\vec{n} dB$$

$$+ \int w_{ib}\phi S_\alpha \mathbf{D}^i_\alpha \nabla(\rho_\alpha w^i_\alpha)\vec{n} dB]]] \cdots\cdots (3.1)$$

where, nel is total number of elements, nd is dimension of the problem, nn is total number of nodes in each element, na is total number of phases excluding soil phase.

Boundary loads of advective and dispersive mass flux can be expressed as follows:

$$\int w_i \rho_\alpha w^i_\alpha \mathbf{K}_\alpha \left(\nabla h_\alpha + \frac{\rho_\alpha}{\rho w}\vec{j}\right) \cdot \vec{n} dB = -\int w_i q^i_{\alpha,h} dB \cdots (3.2)$$

$$\int w_i \phi S_\alpha \mathbf{D}^i_\alpha \nabla(\rho_\alpha w^i_\alpha) \cdot \vec{n} dB = -\int w_i q^i_{\alpha,d} dB \cdots\cdots (3.3)$$

where, $q^i_{\alpha,h}$ is outward normal advective flux, and $q^i_{\alpha,h}$ is outward normal dispersive flux.

The boundary flux is integrated as follows using multidimensional basis functions(Kim, 1989) :

$$f^i_{\alpha,d,i} = \int w_i q^i_{\alpha,d} dB = \sum_{ib=1}^{nb} \langle w_i, N_j \rangle q^i_{\alpha,d,ib} \cdots\cdots (3.4)$$

where, ib is boundary nodal number, nb is total number of boundary nodes, and $f^i_{\alpha,d,i}$ is the dispersive boundary load.

4. STABILITY CRITERIA

The system of equations is very dependent upon the component equations. Careful selection of the step size for space and time, and proper initial conditions, are required to reduce the instability problems related to nonlinearities(Abriola and Rathfelder, 1993). To overcome the instability problems, it is necessary to use variable time and spatial step sizes(Cooley, 1983). The variable time step can be determined from the truncation error. The variable spatial step size requires the algorithm to find a shap advancing front. The gradient of the concentration can indicate the presence of a sharp advancing front. Near this location, a smaller step size is required.

In this study, upstream weighting, variable time step, advanced iteration tehniques, element-wise evaluation of parameters, and mass lumping are used to avoid stability problems.

The methodology developed by Karplus(1958) was applied to insure a stable solution. To provide a simple explanation, a stability analysis of a one-dimensional problem is implemented shown in Fig. 3. Two-and three-dimensional cases and different basis functions can also be analyzed through the expansion of the'following finite element analogue:

$$\frac{1}{6\Delta t}[(C^{n+1}_{i+1} - C^n_{i+1}) + 4(C^{n+1}_i - C^n_i) + (C^{n+1}_{i-1} - C^n_{i-1})]$$
$$+ \frac{V}{2\Delta x}[\varepsilon(C_{i+1} - C_{i-1})^{n+1} + (1-\varepsilon)(C_{i+1} - C_{i-1})^n]$$
$$= \frac{D}{\Delta x^2}[\varepsilon(C_{i+1} - 2C_i + C_{i-1})^{n+1}$$
$$+ (1-\varepsilon)(C_{i+1} - 2C_i + C_{i-1})^n] \cdots\cdots (4.1)$$

After rearranging each term of the above equation in the form of $C^{n+1}_i - C^n_i$, the summation of all the coefficients should be less than 0 to satisfy the stability criteria.

$$\frac{D\Delta t}{\Delta x^2} = \frac{C_r}{P_e} < \frac{1}{3(1-\varepsilon)} \cdots\cdots (4.2)$$

Where, $C_r = V/(\Delta x/\Delta t)$is the Courant number, and $P_e = V/(D/\Delta x)$ is the local Peclet number.

Because the system can be interpreted as the moving coordinate by the velocity component of the total derivative, the migration distance by convective flux should be within the already defined analogue, Therefore, $V < (\Delta x/\Delta t)$, which is same as $C_r < 1$.

The above FEM algorithm is very similar to the finite difference algorithm except for the time derivative, which is evaluated at three different spatial points with the weighting factors 1, 4, and 1. Applying the above technique to the generalized finite difference analogue, the stability condition of generalized FDM becomes:

$$\frac{D\Delta t}{\Delta x^2} = \frac{C_r}{P_e} < \frac{1}{2(1-\varepsilon)} \cdots\cdots (4.3)$$

The numerical analogue of one-dimensional FEM and FDM is shown in Fig. 3.

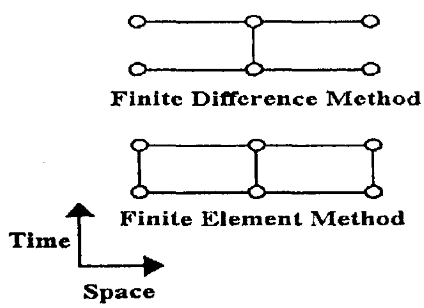


Fig. 3. One dimensional analogs of FEM and FDM.

5. PARAMETER STUDIES

The permeability-saturation-pressure functions of the three phases have been derived from the parametric functions between the capillary pressure and saturation using the two-phase system measurments for calibration(e.g. Leverett and Lewis, 1941; Stone et al., 1970, 1973; Aziz and Settari; 1979; Brooks and Corey, 1964; van Genuchten, 1980). Others have developed an approach which requires only the measured pressure-saturation relations to calibrate relative permeability-saturation-pressure relationships for three-phases(Corey et al., 1956; Parker et al.,e 1987; Parker and Lenhard, 1987;Lenhard et al, 1988a,b,c, 1989, 1991).

In the derivation of macroscopic averaged transport equation in this study, the character of dispersive flux appears as the difference between the microscopic species phase velocity. The dispersion coefficient has the directional property of velocity of each phase and can be different for each component species. The traditional formulation of dispersion coefficient can be expanded for this species dependency as follows(Kim, 1989;Abriolaet al., 1993).

$$D^i_{ij,\alpha} = \alpha^i_{T,\alpha} |\vec{V}_\alpha| \delta_{ij} + (\alpha^i_{L,\alpha} + \alpha^i_{\alpha,T}) \frac{\vec{V}_{i,\alpha}\vec{V}_{j,\alpha}}{|\vec{V}_\alpha|} + D^i_{m,\alpha} \cdots (5.1)$$

where, $D^i_{ij,\alpha}$ is the dipersion coefficient tensor of species in α phase(m/day), $\alpha^i_{T,\alpha}$ and $\alpha^i_{L,\alpha}$ are the transverse and longitudinal dispersivities of species i in α phase(m), $|V\alpha|$ is the absolute velocity, ij is the index for direction, δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ when $i = j$, $\delta_{ij} = 0$ when $i \neq j$), and $D^i_{m,\alpha}$ is the molecular diffusivity.

Based upon the experimental studies which conducted using relatively high flow velocities (e.g., $V_w > 3.5m/d$, Powers et al., 1994), the velocities are more closely associated with forced gradient flow, such as that occurring during a pump and treat remediation effort. Under such conditions, the results clearly demonstrate the invalidity of the local equilibrium assumption for NAPL dissolution in porous media. Observed values of the dissolution rate constant ranged from about $0.1d^{-1}$ to several hundred d^{-1} in the most recent studies(Powers et al., 1994; Imhoff et al., 1994). The specific value depends on strongly on the flow rate and NAPL-pore geometry. In the framework of the present model, the single-component NAPL dissolution rate expression takes the following form:

$$\frac{\partial w^o_w}{\partial t} = k^o_{ow}(w^o_{ws} - w^0_w) \cdots\cdots (5.2)$$

where k^o_{ow} is the NAPL dissolution rate constant $[d^{-1}]$, W^o_{ws} is the mass fraction of the organic species at the aqueous solubility limit.

The equilibrium volatility of a NAPL is governed by its vapor pressure. The present model uses the following dimensionless vapor pressure term:

$$w^o_\alpha = \frac{P^o M^o}{\rho_\alpha RT} \cdots\cdots (5.3)$$

where, P^o is the vapor pressure of the organic compound [pressure], M^o is the molecular weight of the organic compound [M], ρ_α is the density of air $[M_a/U_a]$, R is the gas constant [e. g., J/mol/K], T is the absolute temperature [K].

Raoult's Law applies and the equilibrium mass fraction of each organic species in the vapor phase is assumed to be proportional to its mass fraction in the mixture(Corapcioglu and Baehr, 1987).

$$w^i_\alpha = w^i_o \frac{P^o M^o}{\rho_\alpha RT} \cdots\cdots (5.4)$$

For dilute solutions of an organic species, the equilibrium partitioning of volatile organic chemicals between air and water is descrived by the Henry's Law constant:

$$w_{\alpha}^{o} = H_{aw}^{o} w_{w}^{o} \cdots\cdots (5.5)$$

where H_{aw}^{o} is the dimensionless Henry's Law constant.

For sparingly soluble organic species, the Henry's Law constant is insensitive to concentration, even near the solubility limit of the species. Henry's Law constant data are available for many compounds(Schwarzenbach et al., 1993), and, like vapor pressures, display a wide range of volatility among compounds of environmental interest. Dimensionless values range from about 10^{-5} to 10^{-2}, for PAHs, from about 0.04 to 3, for chlorinated solvents, and from about 1 to 300 for aliphatic hydrocarbons.

The multiphase mass balance equation is transformed as follows to include the nonequilibrium sorption:

$$\sum_{\alpha=1}^{3}\left[\frac{\partial(\phi S_{\alpha}\rho_{\alpha}w_{\alpha}^{o})}{\partial t}\right] + \frac{\partial}{\partial t}((1-\phi)\rho_s w_s^o + \phi S_{wi}\rho_{wi}w_{wi}^{o})$$
$$= \sum_{\alpha=1}^{3}[-\nabla(\phi S_{\alpha}\rho_{\alpha}w_{\alpha}^{o}\vec{V}_{\alpha}) + \nabla(\phi S_{\alpha}D_{\alpha}^{o}\nabla(\rho_{\alpha}w_{\alpha}^{o}))]$$
$$+ \sum_{\alpha=1}^{4}[\phi S(I_{\alpha}^{o} + g_{\alpha}^{o})] \cdots\cdots (5.6)$$

where, ρ_{wi} is the density of the immobile water phase, w_{wi}^{o} is the mass fraction of the organic species in the immobile water phase.

Most intrasorbent diffusion models describe a series of two mass transfer resistances: 1) interphase transfer between the advection-dominated phase and the diffusion-dominated phase, and 2) intraphase transport within the diffusion-dominated phase. The sorbent's capacity for the solute is still dictated by the equilibrium distribution coefficient. A first-order approximation lumps the series of two rate parameters into a single interphase mass transfer rate constant. In the context of the current model, nonequilibrium sorption is an interphase transfer problem that is written as

$$\sum_{\alpha=4}^{5}[\phi S_{\alpha}I_{\alpha}^{o}] = \frac{\partial}{\partial t}((1-\phi)\rho_s w_s^o + \phi S_{wi}\rho wiw_{wi}^{o})$$
$$= k_{wwi}^{o}(\rho_w w_w^o - \rho_{wi}w_{wi}^{o}) \cdots\cdots (5.7)$$

where, k_{wwi}^{o} is the mass transfer rate constant (d^{-1}).

Assuming the equilibrium at the immobile water and solid interface($W_W^o = W_{wi}^o H_{wis}^o$), dilute solutions(density of mobile and immobile water phase is constant), and homogeneous porous media($S_w, S_{wi}, \phi, H_{wwi}^{o}$ are constant), sorption process is expressed as follows:

$$\rho_{wi}\frac{\partial w_{wi}^{o}}{\partial t} = \frac{k_{wwi}^{o}}{\phi S_{wi}R_i}(\rho_w w_w^o - \rho_{wi}w_{wi}^{o}) \cdots\cdots (5.8)$$

where, S_{wi} is the saturation of the immobile water phase (i.e., the fraction of the void space that is immobile water), and R_i is the internal retardation factor.

6. CONCLUSIONS

In this study, the technique of the integrated modeling has been derived from the mass and force balances in a multicomponent multiphase system. The developed model encompasses the migration processes of convection, dispersion, dynamic interfacial mass transfer, and biochemical generation, and the forces of pressure, gravity, interfacial friction, and interfacial momentum transfer.

A comprehensive finite element model was developed to solve the nonlinear transport and constitutive equations of the immiscible fluid flow using multidimensional bilinear elements.

Parameter notations were improved for the fluid conductivity tensor, storage coefficient, dispersion and partition coefficients to facilitate coding. Due to the complexity of the governing equation developed in this study, more general and stable algorithms was provided based upon some of the previous works. The techniques used in the code includes : 1) multidimensional basis and weighting functions, 2) element-wise evaluation of parameters, 3) modified Picard iteration, 4) decoupling of the governing equations, 5) multidimensional evaluation of boundary conditions, and 6) systematic expression of variables with respect to the dimension, species, phase, spatial direction and nodal point.

Even though it was difficult to thoroughly optimize the code for vector processing due to the severe nonlinearities and the recursive relations among process, the vectorization gave excellent results. the computation time after vectorization was only one third of the time required for scalar processing. The following programming techniques were used to facilitate vectorization.

1. The dimension of all arrays was defined in descending order(A(np, ne, na), where, np 〉 ne 〉 na).
2. About 80% of the computation time was spent in the evaluation of the element matrices. Therefore, the element matrices were evaluated over the whole domain, not over the each element, and assembled later. this facilitates vectorization, but increases the storage requirements.
3. In the case of multiple DO-loops, the inner-most DO-loop was for the largest array.
4. The recursive variables were evaluated outside of the DO-loops by using redundant variables.

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