Mathematical Modeling, Numerical Techniques, and Computer Simulation of Flows and Transport in Porous Media

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1. Introduction

Flow of underground water has been studied by hydrologists and soil scientists in connection with applications to both civil and agricultural engineering. The reservoir modeling of multi-phase and multicomponent flows has been used in the petroleum industry for production and recovery of hydrocarbon. Transport of radionuclides into the aquifer has been studied by nuclear engineers in connection to possible leaks from tanks with radioactive materials. Finally, various problems of flows in porous media are related to the design and evaluation of remediation technologies and water quality control.

In the last several decades hydrology and petroleum engineers have become increasingly involved in modeling and computer simulation of flows and transport in underground reservoirs. These efforts have led to development of a wide range of mathematical models for saturated single phase flow, saturated/unsaturated two-phase flow and multi-phase, multicomponent flow and transport. In general, these are systems of nonlinear partial differential equations of convection-diffusion-reaction type. The formulation of the differential model is usually based on the mass conservation principle enhanced with constitutive relations such as the Darcy's and Henry's laws.

In many practical situations the system of equations can be simplified substantially. For example, incompressible fluid flow in fully saturated reservoir is adequately described by a single elliptic equation for the pressure and transport equation(s) for the concentration(s) of the pollutant(s). This model has been successfully used in underground hydrology in the past century.

Driven by the needs for design of technologies for production and recovery of oil and gas the petroleum industry has developed and implemented a variety of compositional models of multi-phase multicomponent flows (see, e.g. [1], [27]). In environmental protection considerations the problems are similar to those of the petroleum industry, but differ in many respects. Here the pressures are much lower, the variety of species is much larger, the topography of the reservoir plays an important role, and the needed accuracy is often very high (especially for the concentration of the pollutants). This requires adequate modeling and accurate numerical techniques. An example of such complex phenomenon is the transport of radionuclides in multiphase groundwater flow in combination with sorption, desorption and radioactive decay [20],[26].

In this paper we present a variety of models in groundwater hydrology that have been used in computer simulation for design of remediation and clean-up technologies. We also discuss the important question of the choice of the approximation method for the corresponding mathematical problem. In fluid reservoirs (aquifer and petroleum reservoirs) there are two imperative practical requirements: the method should conserve the mass locally and should produce accurate velocities (fluxes) even for highly nonhomogeneous media with large jumps in the physical properties. This is the reason that the finite volume method with harmonic averaging of the coefficients has been very popular and successful in computer simulation of flows in porous media. However, when the problem requires accurate description of the topography and the hydrological structure, a more general technique based on the finite element approximation is needed. The mixed finite element method has these properties. Since its introduction by Raviart and Thomas [23] and its implementation by Ewing and Wheeler [17] for flow problems, it has become a standard way of deriving high-order conservative approximations. It should be noted that the lowest-order mixed method realized on rectangles (or parallelepipeds) with certain numerical integration produces cell-centered finite differences with harmonic averaging.

In Section 5 we describe briefly the mixed finite element method for the linearized pressure equation using Raviart-Thomas finite elements. This will lead to a symmetric but indefinite system for the unknown pressure and velocity (flux). Next, we discuss briefly the algorithms involved in the solution of this saddle point type problem and introduce a variant of the classical Uzawa method. This variant was studied recently in [5], [14] and tested on a variety of saddle point problems (see [14]).

Finally, in the last section we discuss the results of numerical simulation of transport of a dense contaminant in a homogeneous water reservoir with a complex three-dimensional reservoir topography.

2. Fluid Flow and Transport Models

In order to establish our notation and terminology we shall use the "naive" approach of mixtures [1]. A mixture is a collection of overlapping continua called constituents. In flow in porous media we shall distinguish two types of mixtures: in one, the segregation among the different constituents occurs at a molecular scale but not at the microscopic scale (the later, characterized by the typical length of the pore

diameter). We shall call such mixtures multi-species or multi-component media. Salt water is a good example. In the second type of mixture, segregation among the constituents occurs at the microscopic level, where the constituents behave as continua, but their small scale motions are inaccessible to direct measurement. These are called multi-phase media. As an example, consider sand with water and air inside. This we call an unsaturated flow regime.

Our goal is to formulate a selection of models that describe accurately various soil processes including coupled water and air phase flows and contaminant transport in both phases. We shall assume that there are two phases water (liquid) and gas. The solid phase is immobile and consolidated (i.e. does not move) and therefore is left out of our considerations. The gas and liquid phases are assumed to be mobile, but immiscible, and the temperature is assumed to be constant.

We assume that the porous media is represented by a polyhedral domain Ω in the three dimensional Euclidean space. For time dependent problems the initial moment is $t = 0$.

The simplest and the most popular model is that of fully a saturated, incompressible porous media. In this case the water (or the liquid) phase occupies the whole pore space and the flow is due to the nonuniform pressure distribution. The mathematical formulation is based on the mass balance equation and Darcy's law (see, e.g. [2], [19]):

$$\begin{aligned} \nabla \cdot (\rho \mathbf{u}) &= F, \\ \mathbf{u} &= -\frac{\mathbf{K}}{\mu}(\nabla p - \rho \mathbf{g}), \end{aligned} \qquad \text{in} \quad \Omega, \tag{2.1}$$

where $\mathbf{u}$ is the volumetric flux of water, F is a source or sink of fluid, ρ is the fluid density, $\mathbf{K}$ is the absolute permeability tensor, μ is the dynamic fluid viscosity, p is the fluid pressure, and $\mathbf{g}$ is acceleration vector due to gravity.

Darcy's law provides a relation between the volumetric flux in the mass conservation equation and the pressure in the fluid. This relation is valid for viscous dominated flows that occur at relatively low velocities.

The transport of a contaminant that is dissolved in the water is described by the following equation:

$$\frac{\partial(\theta c)}{\partial t} + \nabla \cdot (\mathbf{u}c) - \nabla \cdot (\theta \mathbf{D} \nabla c) + \beta \theta c = G(c), \qquad \text{in} \quad \Omega, \quad t > 0. \tag{2.2}$$

Here c is the concentration of the contaminant, $\mathbf{D}$ is the dispersion tensor, β is the reaction rate, $\theta = \phi\rho$, ϕ is the porosity, and G is the source/sink term.

These two equations supplied with appropriate boundary and initial conditions, represent the simplest model of single phase flow and transport in porous media.

An important aspect of the groundwater flow and transport models is the adoption of adequate well models. The wells often play an essential role in simulating the

groundwater flow and for this reason their nature as generators of certain types of flow behavior must be understood very well. A widespread consensus is that the most common type of extraction/injection well used in field applications is one consisting of a screened subsurface region from which fluid is being extracted or injected at a known pump rate. Since the inside of the screened region does not contain porous media, the flow there is determined by the Navier-Stokes equations. A good formulation of the flow model requires coupling Navier-Stokes flow to the Darcy flow outside. However, such a coupling is a very challenging mathematical problem and for this reason various simpler models have been proposed. Perhaps the simplest way of simulating a partially (or fully) penetrating well is to treat the well surface Γ_{well} as an additional boundary where the prescribed pumping rate is distributed in some fashion. One problem, though, is that in general the correct flux distribution is not known. If the flux is assumed to be distributed uniformly, then one can consider this to be a "constant flux" well model. Another popular assumption is that the hydraulic pressure head along the well is constant but unknown. This is often referred to as a "constant head" well model. Mathematically, these models can be given by

$$\int_{\Gamma_{well}} \mathbf{u} \cdot \nu = q, \quad \text{and} \quad p - \rho g z = Const, \tag{2.3}$$

where z is the vertical spatial direction pointing downward, ν is the outward normal vector to the well surface, and g is the acceleration constant due to gravity. The constant head model results in variable extraction rates on the well surface.

Alternatively, much more complex well models based on resolving flow in the interior of the well with some simple differential model with corresponding restrictive assumption for flow inside are also possible, e.g. "bottom hole pressure" model. This model has been very popular in the petroleum industry. In principle, such an approach leads to significant numerical difficulties.

3. Unsaturated Porous Media: Richards Equation

The flow in a system of water and air phases can naturally be described in terms of conservation laws applied to each fluid phase combined with Darcy's law and other empirical material-dependent constitutive relationships. In the unsaturated zone the latter are the capillary pressure and relative permeability as functions of saturation. The following equations for an air-water system are used in the groundwater hydrology [1], [2], [10], [19]:

$$\begin{aligned} \frac{\partial(\phi \rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) &= F_\alpha, \\ \mathbf{u}_\alpha &= -\frac{\mathbf{K} k_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \mathbf{g}), \end{aligned} \qquad \alpha = a,\ w, \tag{3.1}$$

where S_α is the saturation, ρ_α is the density, $\phi(p)$ is the porosity, $\mathbf{u}_\alpha$ is the volumetric flux of phase α, and F_α is the source term. The index α refers to the air (a) and water

(w) phase, respectively. The first equations represent mass conservation of phase α and the second equation is Darcy's law (established experimentally).

Within the groundwater literature, the pressure normally is scaled by the gravity potential function. Equation (3.1) would then be given in terms of the pressure head. This is especially useful when the process allows the elimination of the air-phase equation by the assumption that the air-phase remains essentially at atmospheric pressure. This assumption does not imply that the air phase is stagnant but rather just the opposite, it has a very high mobility [3]. In this case the air-phase mass balance equation is eliminated and the remaining water-phase equation is used to describe the movement of water in the reservoir. This is the well known Richards model (see, e.g. [2], [19]):

$$\begin{aligned} \rho_w\left(\frac{\partial\theta}{\partial t} + S_s\frac{\theta}{\phi}\frac{\partial p}{\partial t}\right) + \rho\frac{\partial\rho}{\partial c}\frac{\partial c}{\partial t} + \nabla\cdot(\rho_w\mathbf{u}_w) &= F_w \\ \mathbf{u}_w &= -\frac{\mathbf{K}k_{rw}}{\mu}(\nabla p - \rho_w\mathbf{g}) \end{aligned} \qquad \text{in } \Omega,\ t>0. \tag{3.2}$$

Here S_s is the specific storativity, $\theta = \rho_w S_w$ is the moisture content with S_w the water saturation, and ϕ is the porosity of the media. This is a nonlinear equation for the unknown pressure since the moisture content θ and the relative permeability k_{rw} depend on the pressure p. The constitutive relationships $\theta = \theta(p)$ and $k_{rw} = k_{rw}(p)$ are established experimentally and then fitted by some functional form (see, e.g. van Genuchten, [25]). The popularity of the van Genuchten fits comes from the fact that they produce smooth functions that are easy to handle numerically. For example, one of the most commonly used functions to model the dependence $\theta = \theta(p)$ is given by

$$\theta(p) = \frac{\theta_s - \theta_r}{[1 + (\delta|H|)^n]^{1-1/n}} + \theta_r. \tag{3.3}$$

Here $H = p/(\rho_0 g)$, ρ_0 is a reference density and θ_s, θ_r, δ and n are fitting parameters.

Similarly, the function $k_{rw} = k_{rw}(p)$ can be given by

$$k_r(p) = R\frac{[1 - (\delta H)^{n-1}(1 + (\delta|H|)^n)^{-m}]^2}{[1 + (\delta|H|)^n]^{m/2}}, \tag{3.4}$$

where R is a fitting parameter and $m = 1 - 1/n$. $H = p/(\rho_0 g)$, δ, and n are the van Genuchten fitting parameters used to characterize $\theta = \theta(p)$.

In addition, functional forms $\mu = \mu(c)$ and $\rho = \rho(p, c)$ may be specified. Here c is the concentration of the most dominant contaminant or some effective concentration obtained by averaging the concentrations of all components.

Equations (3.2)-(3.4) and (2.2) now form the system describing the flow and transport processes in underground reservoirs. Further assumptions of constant water

density and negligible porosity changes lead to simpler forms of equation (3.2) (see, e.g., [19]).

4. Multi-phase, Multi-component Flow and Transport

There are important practical cases when the Richards equation is insufficient to describe adequately the flow and transport processes. Example are vapor extraction systems or soil venting in which there is substantial dynamic interaction between the two phases and the contaminant can be transported both in the air and water phases (see, e.g., [3], [8]). Another example where the air phase has to be solved explicitly is the presence of injection wells which pump fluid into the porous media at high pressure. In such situations the coupled nonlinear system (3.1) for the air-water complex has to be solved.

Next, we present the two-phase fluid flow and contaminant transport model using the well known fractional flow formulation coupled with a transport equation [2], [3], [19]. This approach results in a mathematical problem which is well behaved when solved numerically. The fractional flow formulation involves a global pressure p and total velocity $\mathbf{u}$. This provides a two-phase water (w) and air (a) flow model which is described by the following equations [10], [11]:

$$\begin{aligned} C(p,S_w)\frac{\partial p}{\partial t} + \nabla\cdot\mathbf{u} &= f(p,S_w), \\ \mathbf{u} &= -\mathbf{K}\lambda(\nabla p - \mathbf{G}_\lambda), \end{aligned} \qquad \text{in } \Omega,\ t>0, \tag{4.1}$$

$$\frac{\partial(\phi\rho_w S_w)}{\partial t} + \nabla\cdot\rho_w(f_w\mathbf{u} - \mathbf{K}\lambda_a f_w \delta\rho\mathbf{g} - \mathbf{D}(S_w)\cdot\nabla S_w) = F_w, \ \text{ in } \Omega,\ t>0. \tag{4.2}$$

The global pressure and total velocity are defined by [10], [11]:

$$p = \frac{1}{2}(p_w + p_a) + \frac{1}{2}\int_{S_c}^{S_w} \frac{\lambda_a - \lambda_w}{\lambda}\ \frac{dp_c}{d\xi}d\xi \quad \text{and} \quad \mathbf{u} = \mathbf{u}_w + \mathbf{u}_a. \tag{4.3}$$

Here

$$C(p,S_w) = \frac{\phi S_w}{\rho_a}\frac{d\rho_a}{dt}, \tag{4.4}$$

$$f(p,S_w) = (F_a - \mathbf{u}_a\cdot\nabla\rho_a - \phi S_a\frac{\partial\rho_a}{\partial t})/\rho_a + (F_w - \mathbf{u}_w\cdot\nabla\rho_w - \phi S_w\frac{\partial\rho_w}{\partial t})/\rho_w, \tag{4.5}$$

$\lambda = \lambda_w + \lambda_a$ is the total mobility, and $\lambda_\alpha = \frac{k_{r\alpha}}{\mu_\alpha}$, $\alpha = w, a$, is the mobility for water and air, where $k_{r\alpha}$ is the relative permeability. The capillary pressure p_c is given by $p_c = p_a - p_w$. The gravity forces $\mathbf{G}_\lambda$ and capillary diffusion term $\mathbf{D}(S)$ are expressed as

$$\mathbf{G}_\lambda = \frac{\lambda_w\rho_w + \lambda_a\rho_a}{\lambda}\ \mathbf{g} \qquad \text{and} \qquad \mathbf{D}(S) = -\mathbf{K}\lambda_a f_w\frac{dp_c}{dS}.$$

The phase velocities for water and air, which are needed in transport calculations, are given by:

$$\begin{aligned} \mathbf{u}_w &= f_w \mathbf{u} + \mathbf{K}\lambda_a f_w \nabla p_c - \mathbf{K}\lambda_a f_w \delta\rho \mathbf{g}, \\ \mathbf{u}_a &= f_a \mathbf{u} - \mathbf{K}\lambda_w f_a \nabla p_c + \mathbf{K}\lambda_w f_a \delta\rho \mathbf{g}, \end{aligned} \tag{4.6}$$

where $f_\alpha = \lambda_\alpha/\lambda$, $\alpha = w, a$, and $\delta\rho = \rho_a - \rho_w$. To complete the model, we assume constitutive relations between capillary pressure and saturation and also between relative permeabilities and saturation, i.e.

$$p_c = p_c(S_w) \quad \text{and} \quad k_{r\alpha} = k_{r\alpha}(S_w).$$

Notice, that the phase velocity for air is given by (4.6) even if the Richards approximation is used.

In conjunction with the above flow model we consider transport equations based on a kinetic phase transfer. The rate of contaminant transfer from one phase to the other is determined by the degree of disequilibrium, a kinetic phase transfer coefficient and the water content. Then the transport of contaminant is described by the following equations [1], [3]:

$$\begin{aligned} \frac{\partial(\theta_w c_w)}{\partial t} + \nabla\cdot(\mathbf{u}_w c_w) - \nabla\cdot(\theta_w \mathbf{D}_w \nabla c_w) + \beta_w \theta_w c_w &= G_w, \quad \text{in } \Omega, \quad t > 0, \\ \frac{\partial(\theta_a c_a)}{\partial t} + \nabla\cdot(\mathbf{u}_a c_a) - \nabla\cdot(\theta_a \mathbf{D}_a \nabla c_a) + \beta_a \theta_a c_a &= G_a, \quad \text{in } \Omega, \quad t > 0. \end{aligned} \tag{4.7}$$

Here c_α is the concentration of the pollutant in phase α, $\theta_\alpha = \phi S_\alpha$, $\mathbf{D}_\alpha$ is the dispersion tensor for phase α, β_α is the reaction rate for phase α, $\mathbf{u}_\alpha$ is the volumetric flux of phase α, and G_α is the source/sink term, $\alpha = a, w$. Similarly to the Richards model, constitutive relations $\mu = \mu(c)$ and $\rho = \rho(p, c)$ may be specified here.

In the case of radionuclide transport, c_w and c_a are vectors of the concentrations of various radionuclides in the water and air phases, respectively. Then one should add a set of ordinary differential equations to the above model that describes the change of the corresponding concentrations in the rock as a consequence of the processes of sorption and desorption (see, e.g. [26]).

The boundary conditions are an important element of the above model. Standard types of boundary conditions, namely Dirichlet, Neumann and Robin, are assumed for the transport equations (4.7). The pressure-saturation formulation of the flow model (4.1)-(4.2) deserves special attention.

Let the boundary Γ of Ω be partitioned into non-overlapping parts Γ_i, $i = 1, 2, 3$. Then boundary conditions for (4.1) can be given by a combination of the following expressions:

$$p = p_\Gamma(x, t), \qquad x \in \Gamma_1, \quad t > 0, \tag{4.8}$$

$$\mathbf{u}\cdot\nu + b(x, t, S_w)p = G_\Gamma(x, t, S_w), \qquad x \in \Gamma_2, \quad t > 0, \tag{4.9}$$

$$\mathbf{u}_w \cdot \nu + b_w(x,t,S_w)p = G_w(x,t,S_w), \quad x \in \Gamma_3, \quad t > 0, \tag{4.10}$$

where ν is the outward normal vector to the corresponding boundary part and $p_\Gamma(x,t)$, $b(x,t,S_w)$, $G_\Gamma(x,t,S_w)$, $b_w(x,t,S_w)$, and $G_w(x,t,S_w)$ are given functions.

We note that incorporating different well models may result in additional boundary conditions for this system of equations. For example, the constant head well model (2.3) normally results in a boundary condition of the form

$$\int_{\Gamma_{well}} \mathbf{u} \cdot \nu = q(t), \quad \text{and} \quad p - \rho g z = Const(t), \quad \text{on} \quad \Gamma_{well}, \quad t > 0,$$

where Γ_{well} is the well surface and $Const(t)$ is the unknown value that actually may change in time.

A corresponding set of boundary condition for the saturation equation must be specified. From a physical point of view, a Dirichlet condition for the saturation imposed on the boundary Γ makes very good sense. Of course, boundary conditions of the form (4.8)–(4.10) make a perfect mathematical sense here but their physical meaning is not necessarily well defined.

Since the total pressure and velocity are not physical quantities, boundary conditions involving only these variables may not be available for many applications. Most commonly, the boundary conditions for the two phase system involve variables that are nonlinear functions of the boundary values of the physical quantities in the original two-pressure formulation [3], e.g. $\boldsymbol{u}_w$ in equation (4.10). This means that we have to iterate on the boundary conditions as a part of the solution process.

5. Discretization Technique

Three main factors have played an important role in selecting our discretization strategy: (a) the mass conservation expressed by the differential equations; (b) the geometry of the domain; (c) nonlinearities in the model and their linearization. There are nonlinearities on multiple levels in the coupled flow and transport model (4.1)-(4.7): within each of the equations, between the pressure and saturation equations, and between the pressure and transport equations. One way of solving this system is to first linearize each equation by lagging in time the setup of the coefficients in order to get an initial guess. After that a Picard or Newton iteration can be applied in order to resolve the non-linearities. Such an approach is used successfully in [3] in the case of unsaturated flows. Other approaches to linearization are discussed in [10] and [15].

The mathematical nature of the transport (4.7), saturation (4.2) and pressure (4.1) equations is different and specific methods for their approximation should be considered. Typically, the transport and the saturation equations are convection dominated and thus special care should be taken in their discretization. Also, the diffusion terms there are small but important and cannot be neglected. On the other hand, the pressure equation has a strong elliptic part and this fact should influence the choice of the discretization method.

Based on these observations, we have used two types of finite element approximations: the standard conforming Galerkin method and the mixed method. Advantages

of the former are its simplicity, smaller number of unknowns, allowance for isoparametric techniques for arbitrary shaped domains, and availability of a vast variety of efficient methods for solving the resulting system of linear equations. These features are particularly important for three-dimensional problems. Combined with upstream weighting, Godunov type approximations or Riemann solvers such discretizations can be used for the transport and the saturation equations (for a combination with the mixed method, see, e.g. [18]). An enhanced performance results from the use of logically rectangular grids. This is the approximation method we use for the saturation and transport equations.

Among the disadvantages of the conforming discretizations are the lack of local mass conservation of the numerical model and some difficulties in computing the phase velocities needed in the transport and saturation equations. The straightforward numerical differentiation is far from being justifiable in problems formulated in highly heterogeneous medium with complex geometry. On the other hand, the mixed finite element method [7] offers an attractive alternative. In fact, this method conserves mass cell by cell and produces a direct approximation of the two variables of interest – pressure and velocity. Below we explain briefly the mixed finite element method for the pressure equation.

To describe the mixed method we introduce two Hilbert spaces. Let

$$W = L^2(\Omega), \qquad \boldsymbol{V} = \left\{ \boldsymbol{\varphi} \in L^2(\Omega)^3,\ \nabla \cdot \boldsymbol{\varphi} \in L^2(\Omega) \right\},$$

and let the space $\boldsymbol{V}$ be equipped with the norm $\| \boldsymbol{\varphi} \|_{\boldsymbol{V}} = (\| \boldsymbol{\varphi} \|^2 + \| \nabla \cdot \boldsymbol{\varphi} \|^2)^{1/2}$. The inner product and the norm in $L^2(\Omega)$ are denoted by $(\cdot, \cdot)$ and $\| \cdot \|$, respectively. For the sake of simplicity, $(\cdot, \cdot)$ and $\| \cdot \|$ are also used as the inner product and norm, respectively, in the product space $L^2(\Omega)^3$.

The pressure equation (4.1) is written in the following mixed weak form: find $(p, \mathbf{u}) \in W \times \boldsymbol{V}$ such that

$$\begin{aligned} &(A\mathbf{u}, \boldsymbol{\varphi}) - (p, \nabla \cdot \boldsymbol{\varphi}) = (\mathbf{G}_\lambda, \boldsymbol{\varphi}), && \forall\ \boldsymbol{\varphi} \in \boldsymbol{V},\ t > 0, \\ &(C(p, S_w)p_t, \psi) + (\nabla \cdot \mathbf{u}, \psi) = (f(p, S_w), \psi), && \forall\ \psi \in W,\ t > 0, \\ &p(0) \in L^2(\Omega) \quad \text{is the given initial pressure.} \end{aligned} \tag{5.1}$$

Here $p_t = \partial p / \partial t$ and $A = (\mathbf{K}\lambda)^{-1}$. We note that A is always symmetric and positive definite which leads to a well defined problem. This is in contrast to (3.1) where the relative permeability $k_{r\alpha}$ vanishes when the phase α is absent in some subregion of Ω. We note that if there were nonhomogeneous boundary conditions on $\partial\Omega$ they should be added to the right hand side $(f(p, S_w), \psi)$. Corresponding changes in the bilinear forms in the left hand side should be introduced in the case of Robin boundary conditions. Obviously, (5.1) forms a nonlinear problem. To solve it one can use Picard linearization (see, e.g., [10]) or any other feasible approach.

We triangulate the domain Ω in tetrahedra with characteristic diameter h. Next we introduce the finite element spaces $W_h \subset W$ and $\boldsymbol{V}_h \subset \boldsymbol{V}$ of piece-wise polynomials with respect to the triangulation and time discretization $t_n = n\Delta t,\ n = 0,\ 1, \ldots$. The mixed finite element approximation $(P^n, \boldsymbol{U}^n) \in W_h \times \boldsymbol{V}_h$ of $(p(t_n), \mathbf{u}(t_n)) \in$

$W \times \boldsymbol{V}$ is the solution of the following problem:

$$\begin{aligned} &(A^n \boldsymbol{U}^n, \boldsymbol{\varphi}_h) - (\nabla \cdot \boldsymbol{\varphi}_h, P^n) = (\mathbf{G}^n_\lambda, \boldsymbol{\varphi}_h), && \forall\ \boldsymbol{\varphi}_h \in \boldsymbol{V}_h, \\ &\frac{1}{\Delta t}(C^n(P^n - P^{n-1}), \psi_h) + (\nabla \cdot \boldsymbol{U}^n, \psi_h) = (f^n, \psi_h), && \forall\ \psi_h \in W_h, \\ &P^0 \in W_h \quad \text{is expressed through given initial data.} \end{aligned} \tag{5.2}$$

This is an implicit in time Euler approximation of nonlinear problem (5.1) which can be solved by Picard or Newton iterations. Obviously, one can formulate easily the Crank-Nicolson scheme.

To ensure the existence and optimal convergence of the solution of the linearized version of the above formulation, we assume that

$$\nabla \cdot \boldsymbol{V}_h \subset W_h$$

and there exists a linear operator $\boldsymbol{\Pi}_h$: $\boldsymbol{V} \to \boldsymbol{V}_h$ such that

$$\nabla \cdot \boldsymbol{\Pi}_h = Q_h \nabla \cdot . \tag{5.3}$$

Here, the operator $Q_h :\ W \to W_h$ is the L^2-projection, i.e.,

$$(\psi - Q_h \psi, \psi_h) = 0, \quad \forall\ \psi \in W, \psi_h \in W_h.$$

The identity (5.3) guarantees that the classical *inf-sup* condition is satisfied. Examples of spaces of piece-wise polynomials that satisfy the conditions stated above are the triangular and rectangular Raviart-Thomas elements from [23] and the tertahedral elements of Nedelec [22] (for other examples see [7]). Our implementation is based on partition of the domain on tetrahedra and using the lowest-order Raviart-Thomas elements that involve piece-wise constant pressure (see, e.g. [23]).

The resulting system of linear equations has the form of a saddle point problem defined on a pair of finite-dimensional spaces W_h and $\boldsymbol{V}_h$:

$$\begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{U}^n \\ P^n \end{pmatrix} = \begin{pmatrix} F \\ G \end{pmatrix}, \tag{5.4}$$

where $F \in \boldsymbol{V}_h$ and $G \in W_h$ are given and $P^n \in W_h$ and $\boldsymbol{U}^n \in \boldsymbol{V}_h$ represent the unknown approximate solution on the time level t_n. Here $\mathbf{A} : \boldsymbol{V}_h \mapsto \boldsymbol{V}_h$ is a linear, symmetric, and positive definite operator. In addition, the linear map $\mathbf{B}^T : W_h \mapsto \boldsymbol{V}_h$ is the adjoint of $\mathbf{B} : \boldsymbol{V}_h \mapsto W_h$. $\mathbf{D} : W_h \mapsto W_h$ is either $\frac{1}{\Delta t}\mathbf{M}$ with $\mathbf{M}$ similar to the mass matrix in W_h for time dependent problems or $\mathbf{0}$, for steady state problems. The existence and uniqueness of a solution is guaranteed by the fact that the pair of spaces $(W_h, \boldsymbol{V}_h)$ satisfies the *inf-sup* condition of Babuska-Brezzi [7].

This is an indefinite system with a large number of unknowns. Such a type of system is more difficult to solve compared with the definite systems. However, the popularity of mixed methods has increased considerably as a consequence of the progress made in the recent years in developing efficient methods for solving these equations (see, e.g. [4], [5], [12], [24]).

The saturation equation has more hyperbolic nature and should be treated with related techniques (see, e.g. [1]). It exhibits features of a hyperbolic conservation law

and techniques based on the method of characteristics, Rieman solvers and/or other Godunov type approximations are widely used in its solution. For a survey of various methods and discussion concerning their construction, analysis, and performance related to petroleum applications we refer to [1]. In groundwater applications these equations have been effectively resolved using the modified method of characteristics (MMOC) [13], [16] or the related ELLAM method [3], [9]. These methods can be viewed as special time-stepping procedures that can be combined with any spatial discretization.

MMOC gives rise to a symmetric discrete model which can be effectively solved by iterative methods. However, this method requires accurate approximation of the velocity in order to accurately follow the characteristics. For this reason combinations of MMOC with mixed discretizations often lead to better numerical models.

6. Iterative Methods

Because of significant progress made in developing iterative techniques for systems coming from Galerkin discretizations, we shall not concentrate on this issue. We only mention that domain decomposition preconditioners are particularly useful when the models are implemented on distributed parallel computers [6].

The indefinite systems resulting from mixed finite elements are much more difficult to solve iteratively. In general, the properties of the discrete operators involved in the definition of the system must be understood well in order to design an efficient iterative solution scheme. For example, Raviart-Thomas pairs of finite dimensional spaces produces a well conditined operator $\mathbf{A}$, whereas the Schur complement operator $\mathbf{D} + \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$ exhibits a condition number growth like h^{-2}, where h is the discretization parameter. It is well known that in our setting $\mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$ behaves like a discretization of a second order elliptic operator.

A standard approach used in [17] to solve (5.4) is to perform Gaussian block elimination and obtain the reduced system

$$(\mathbf{D} + \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T)P^n = \mathbf{B}\mathbf{A}^{-1}F - G. \tag{6.1}$$

The classical Uzawa algorithm is a linear iteration for solving (6.1). Alternatively, one can apply preconditioned conjugate gradient to (6.1). A disadvantage of these approaches is that they require the action of $\mathbf{A}^{-1}$ which reduces substantially the efficiency. The inexact Uzawa algorithm which avoids the evaluation of $\mathbf{A}^{-1}$ is defined by

Algorithm [Inexact Uzawa] For $\boldsymbol{U}_0^n \in \mathbf{V}_h$ and $P_0^n \in W_h$ given, the sequence $\{(\boldsymbol{U}_i^n, P_i^n)\}$ is defined, for $i = 1, 2, \ldots,$ by

$$\begin{aligned} \boldsymbol{U}_{i+1}^n &= \boldsymbol{U}_i^n + \mathbf{Q}_A^{-1}\left(F - \left(\mathbf{A}\boldsymbol{U}_i^n + \mathbf{B}^T P_i^n\right)\right), \\ P_{i+1}^n &= P_i^n + \mathbf{Q}_B^{-1}(\mathbf{B}\boldsymbol{U}_{i+1}^n - \mathbf{D}P_i^n - G). \end{aligned} \tag{6.2}$$

Here $\mathbf{Q}_A$ is a symmetric and positive definite preconditioner for $\mathbf{A}$ and is easy to invert. Similarly, $\mathbf{Q}_B$ is a preconditioner for $\mathbf{D} + \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$. Recent convergence results for the inexact the Uzawa algorithm [5] show that under the assumption of

appropriately scaled preconditioners $\mathbf{Q}_A$ and $\mathbf{Q}_B$ this method is guaranteed to converge. It is worth mentioning that there are efficient preconditioners that are scaled appropriately by default. For example, multigrid is automatically scaled properly according to the theory of the inexact Uzawa algorithms whereas a scaling constant must be computed for the incomplete Cholesky factorization.

The conjugate residual method applied to (5.4) is another approach to the solution of this problem. The two level iteration implementation considered in [24] suggests that due to the nonlinearity of the outer iteration the accuracy of the inner solve should be increased considerably for stability. This, however, increases the computational cost of the algorithm.

The positive definite reformulation of (5.4) suggested in [4] is a good method for solving the indefinite problem. This approach utilizes preconditioners for $\mathbf{A}$ and $\mathbf{D} + \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$ and results in a positive definite system which can be solved efficiently by conjugate gradient. However, the preconditioner for $\mathbf{A}$ must be properly scaled. This scaling factor is either known *a priori* or can be obtained by employing computationally cheap procedures for estimating the largest eigenvalue, such as the power method. In general, the linear iteration corresponding to the inexact Uzawa methods converges slower than the conjugate gradient method just described. However, recent numerical investigations by Elman [14] show that the inexact Uzawa algorithm is very competitive computationally. In addition, this method may be advantageous when implemented on distributed memory parallel computers since inner products are not required.

The hybrid mixed formulation [7] provides yet another way for computing the solution to (5.4). The idea behind this method is to impose continuity of the normal components of the velocity at the inter-element interfaces by Lagrange multipliers. From a computational point of view, the main benefit in this formulation is in the fact that the resulting system of linear equation can be reduced to a system for the multipliers which is symmetric and positive definite. The condition number of the latter system is like $O(h^{-2})$ and should be preconditioned. Using equivalence arguments, a domain decomposition preconditioner for this problem is constructed in [12].

As we mentioned earlier, adopting wells in the groundwater flow model leads to certain numerical difficulties that have to addressed. For example, when the simple well model (2.3) is considered, the existing groundwater literature suggests an iterative technique for solving the resulting system of equations based on a a sequence of refined guesses to the unknown constant until the pump rate is achieved. This is a very inefficient way to solve this problem. A much better method can be implemented by imposing the condition of constant (but unknown) pressure directly into the finite element space. Often it is convenient to introduce Lagrange multipliers in order to solve for the unknown flux distribution on the well surface. We note that this approach leads to saddle point problem even in the case when a hybrid mixed formulation is adopted as a method for solving the original indefinite problem. In cases where the number of wells is relatively large (say, more than five), forming the corresponding Schur complement is a very inefficient approach. Thus, iterative

techniques for saddle point problems are useful in such situations. In particular, the inexact Uzawa algorithm (6.2) could be very attractive for solving such problems.

7. Numerical Simulations

In this section we present some of our experience in developing computer simulators based on the models described above. Clearly, most interesting and difficult are three dimensional transient problems and we shall discuss some issues related to such problems.

The approach we have taken in defining the triangulation of the computational domain is based on introducing first an underlying logically rectangular grid. Such grid offers perhaps the most economical way to maintain a simple data structure and to build finite element approximations with minimal number of unknowns. It essentially simplifies many coding issues and yet allows complex geometries to be handled. In fact, our computational grid can be as complex as any reasonable union of logically rectangular structures including toroidal or L-shaped domains.

The basic logically rectangular grid is used for the Galerkin finite element method. Further, to define the mixed method each grid cell is split into five tetrahedra. When the lowest-order Raviart-Thomas spaces are used, one pressure and four velocity unknowns are attached to every tetrahedron in the grid. It is clear that the numerical solution of such models requires extensive memory and CPU resources. In our opinion, only supercomputers are capable of solving these numerical model in reasonable time. We have experimented primarily on distributed memory architectures such as Intel's Paragon.

A domain decomposition approach is used in order to utilize these machines. The original computational domain is decomposed into a set of logically rectangular structures each of which is attached to a single processor. Then a corresponding parallel algorithm for solving the problem is applied.

The system for remote procedure calls (IPX), developed at the Brookhaven National Laboratory [21], has been used for the parallelization of our computer codes. This system provides the user with the ability to write parallel codes in a style that is very close the the common serial style of writing numerical codes and for this reason reduces considerably the complexity of the development software for distributed architectures. In addition, the resulting software is independent of the vendor supplied primitives for parallel processing which is important for the portability. Another interesting feature of IPX is that it can unite the exchange of data and a method of its processing among the computing nodes which leads to more enhanced software environment for creating parallel programs.

At the end of the section we give some computational results from a simulation of groundwater problem. The application is the transport of a very dense contaminant penetrating into an aquifer. This models the following situation: a chemical waste has been dumped in a given area on the surface of the aquifer. A selected portion of the aquifer is shown on Figures 1 and 2. In Figure 2 the lighter spot on the upper corner of the reservoir represents the area covered by the waste. The rainfall dissolves the chemical producing a very dense contaminant which moves through the

unsaturated zone to the saturated zone of homogeneous porous medium. There are no wells or other features that can change dramatically the pressure in the porous media. In this combined process the unsaturated/saturated flow is adequately described by Richards equation (3.2) and the transport of the miscible contaminant is modeled by Equation (2.2). We stress two aspects that play an important role in this process. First, the bedrock is practically impermeable and has a highly irregular geometry which is clearly shown on Figures 1 and 2. The bedrock elevations were provided by field personnel from seismic measurements. Secondly, the contaminant is very dense which make the term $\rho\frac{\partial\rho}{\partial c}\frac{\partial c}{\partial t}$ in Richards equation (3.2) act as a strong forcing term in addition to the existing gravity forces. This produces a velocity that has dominant vertical (downward) component. Thus, the contaminant is transported mostly downward and after reaching the bedrock it follows the bottom shape. This is clearly seen on Figure 3 where the isosurface of the concentration level 80 % is shown.

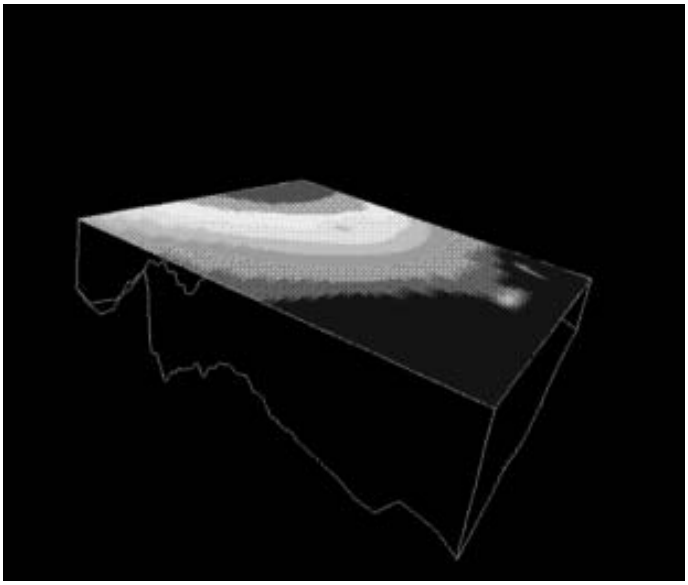

Figure 1. 3-D simulation: pressure distribution at the surface.

The computational results show very interesting phenomena of contaminant distribution with the time progressing, due to the combination of forces driving the process, the geometry of the domain and the properties of the medium. They are in good agreement with experimental results obtained by measuring concentrations in real sites with similar conditions. For example, field tests conducted at the site

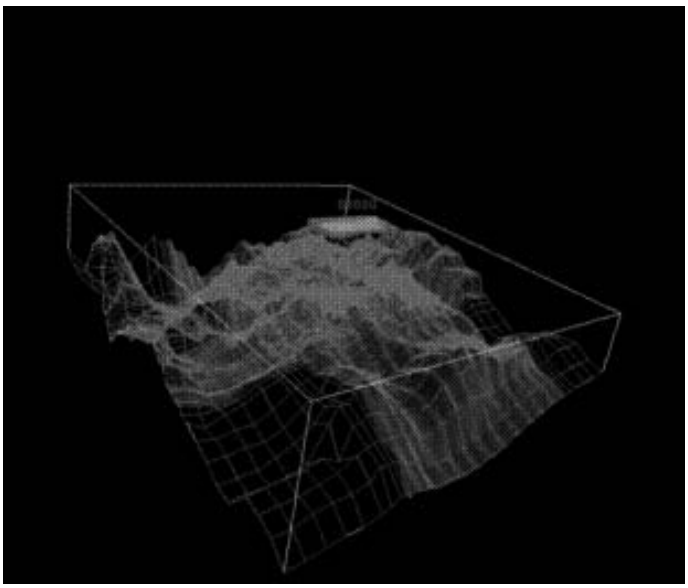

Figure 2. 3-D simulation: bedrock and contaminant leakage spot.

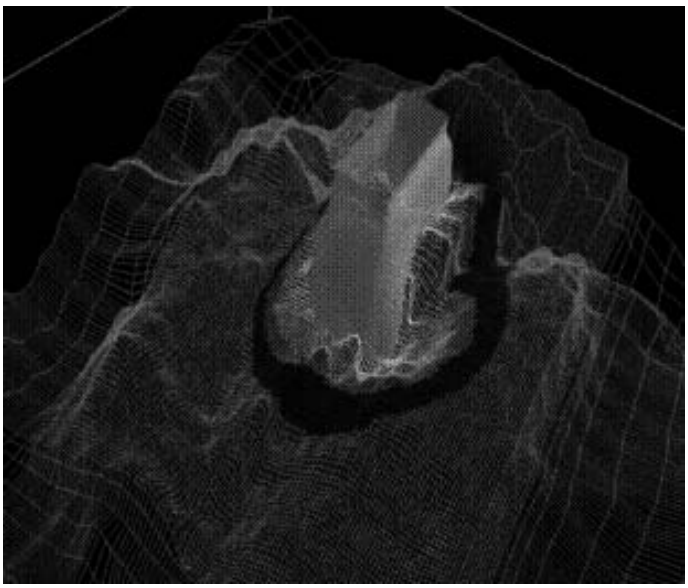

Figure 3. 3-D simulation: isosurface of the concentration level 80% after 2000 days.

indicated contaminant movement against the groundwater flow direction. Our simulation was essential in understanding why the pollutant flowed upstream but "down" the bedrock slope.

The simulation of the flow and transport problem presented in a domain with $136 \times 128 \times 10$ grid cells was performed on a 56-processor Intel Paragon. The properties

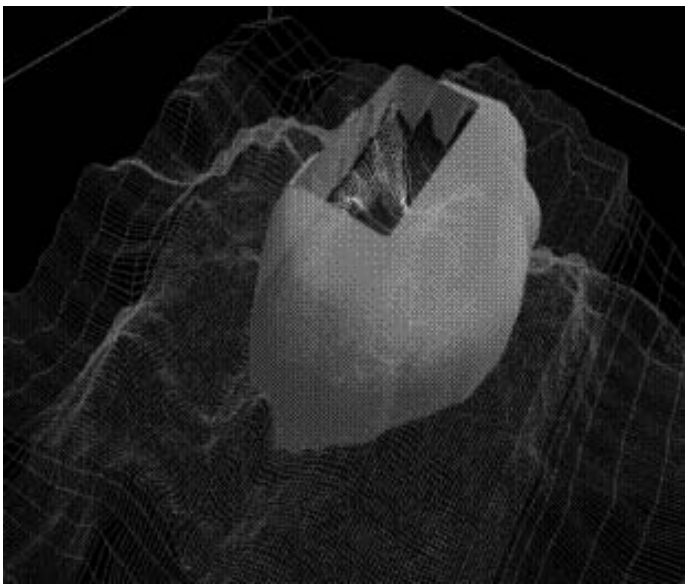

Figure 4. 3-D simulation: isosurface of the concentration level 10% after 2000 days.

of the porous medium were specified with respect to this grid. The time step Δt was 4 days and the simulation period was 15 years.

8. Acknowledgments

This research has been partially supported by PICS project on Groundwater modeling funded by DOE contract, DE–FG05–92ER25143.

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