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Invited Paper

Three-dimensional numerical codes for simulating groundwater contamination: FLOW3D, flow in saturated and unsaturated porous media

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Abstract

In this paper we describe the numerical code for a three-dimensional groundwater flow model. The model is developed for the case of variably saturated porous media, applicable to both the unsaturated (soil) zone and the saturated (groundwater) zone. The governing equation is nonlinear, and is linearized using either Picard or Newton iteration. The large sparse systems of linear equations generated by the finite element discretization are solved using efficient preconditioned conjugate gradient-like methods. Tetrahedral elements and linear basis functions are used for the discretization in space, and a weighted finite difference formula is used for the discretization in time. The code handles: temporally and spatially variable boundary conditions, including seepage faces and evaporation/precipitation inputs; heterogeneous material properties and hydraulic characteristics, including saturated conductivities, porosities, and storage coefficients; and various expressions to describe the moisture content-pressure head and relative conductivity-pressure head relationships. The model solves for nodal pressure heads, and uses these values to compute the water saturations and velocities over the flow domain. The water saturation and velocity values can be used as input to the LEA3D and NONLEA3D transport codes, which are described in a companion paper.

Introduction

Virtually all sectors of society are affected by water quality degradation. Tourism declines when lakes, streams, and coastal areas become polluted; farmland is abandoned when irrigation waters drawn from aquifers are depleted; human health is endangered when drinking water supplies become contaminated, and so on. Since groundwater constitutes, in the global hydrosphere, the most important source of freshwater, understanding the processes of water flow and contaminant transport in these subsurface repositories is an urgent problem.

Mathematical models of flow and transport processes in porous media can be effectively used to investigate the migration and fate of contaminants in soils and groundwater. The models are based on the partial differential equations of fluid and solute continuity, and can be solved numerically by finite element and other methods. With finite element techniques it is relatively easy to simulate irregular three-dimensional domains with complex boundary conditions, such as those commonly found in real applications.

This is the first of two papers describing a set of complementary three-dimensional finite element models for simulating saturated and unsaturated flow and equilibrium and nonequilibrium transport in porous media. In this paper we describe the features of the flow code, FLOW3D, which include:

- ◇ Choice of several functions to describe the moisture content-pressure head and relative conductivity-pressure head relationships, along with various options for differentiation of these constitutive relations;
- ◇ Handling of heterogeneous material and hydraulic properties;
- ◇ Automatic 3-D mesh generation from a 2-D surface grid;
- ◇ Handling of temporally and spatially variable boundary conditions, including seepage faces and evaporation/precipitation inputs;
- ◇ Choice of Picard or Newton iteration for the nonlinear equation;
- ◇ Choice of several preconditioned conjugate gradient-like methods to solve the large sparse systems resulting from Picard or Newton linearization;
- ◇ Dynamic time step control, with a back stepping feature to reduce the time step when convergence fails;
- ◇ Output of water saturation and velocity values for use as input to the transport codes.

Richards' Equation and Soil Constitutive Relations

Flow in unsaturated and variably saturated porous media is governed by Richards' equation, which may be written as (Philip [1])

$$\frac{\partial}{\partial x_i}\left[k_{ij}k_{rw}(S_w)\left(\frac{\partial \psi}{\partial x_j}+\zeta_j\right)\right]=\sigma(S_w)\frac{\partial \psi}{\partial t}-q \qquad (1)$$

where the indices i and j denote summation over the three coordinate dimensions $(i,j=1,2,3)$, x_i is the ith Cartesian coordinate $(x_3=z)$, k_{ij} is the saturated hydraulic conductivity tensor, k_{rw} is the relative hydraulic conductivity, $S_w = \theta/n$ is the water saturation, θ is the volumetric water content, n is the porosity of the medium, ψ is the pressure head, $\zeta_1 = \zeta_2 = 0$, $\zeta_3 = 1$, σ is the general storage term, t is time, and q represents distributed source or sink terms (volumetric flow rate per unit volume).

Equation (1) is highly nonlinear due to pressure head dependencies in the storage and conductivity terms. These terms can be modeled using various constitutive or characteristic relations describing the soil hydraulic properties. Parameter IVGHU in the FLOW3D code allows the user to choose between the following four families of curves:

IVGHU = 0 (van Genuchten and Nielsen [2]):

$$\begin{aligned} \theta(\psi) &= \theta_r + (\theta_s - \theta_r)[1+\beta]^{-\mu} & \psi &< 0 \\ \theta(\psi) &= \theta_s & \psi &\geq 0 \end{aligned} \tag{2}$$

$$\begin{aligned} k_{rw}(\psi) &= (1+\beta)^{-5\mu/2}\left[(1+\beta)^{\mu} - \beta^{\mu}\right]^2 & \psi &< 0 \\ k_{rw}(\psi) &= 1 & \psi &\geq 0 \end{aligned} \tag{3}$$

where θ_r is the residual moisture content, θ_s is the saturated moisture content, $\beta = (\psi/\psi_s)^{\eta}$, ψ_s is the capillary or air entry pressure head value, η is a constant, and $\mu = 1 - 1/\eta$. The corresponding general storage term is

$$\sigma(S_w) = S_w S_s + n\frac{dS_w}{d\psi} \tag{4}$$

where S_s is the specific elastic storage of the porous medium.

IVGHU = 1 (Paniconi *et al.* [3]):

$$\begin{aligned} \theta(\psi) &= \theta_r + (\theta_s - \theta_r)[1+\beta]^{-\mu} & \psi &< \psi_o \\ \theta(\psi) &= \theta_r + (\theta_s - \theta_r)[1+\beta_o]^{-\mu} + S_s(\psi - \psi_o) & \psi &\geq \psi_o \end{aligned} \tag{5}$$

where ψ_o is a continuity parameter and $\beta_o = \beta(\psi_o) = (\psi_o/\psi_s)^{\eta}$. $k_{rw}(\psi)$ is as in equation (3), and the general storage term is $\sigma = d\theta/d\psi$.

IVGHU = 2 (Huyakorn *et al.* [4]):

$$\begin{aligned} S_e(\psi) &= [1 + \epsilon^{\eta}(\psi_a - \psi)^{\eta}]^{-\gamma} & \psi &< \psi_a \\ S_e(\psi) &= 1 & \psi &\geq \psi_a \end{aligned} \tag{6}$$

$$k_{rw}(\psi) = k_{rw}\left(S_e(\psi)\right) = S_e^{\mu} \tag{7}$$

where the water saturation has been expressed in terms of effective saturation S_e, in the form $S_w(\psi) = (1 - S_{wr})S_e(\psi) + S_{wr}$, S_{wr} $(= \theta_r/n)$ is the residual water saturation, ψ_a is the air entry pressure, and ϵ, η, γ, and μ are constants. The general storage term is as in equation (4).

IVGHU = 3 (Huyakorn *et al.* [4]):

$$k_{rw}(\psi) = 10^{G(S_e(\psi))} \tag{8}$$

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where $G(S_e) = aS_e^2 + (b - 2a)S_e + a - b$, and a and b are constants. $S_e(\psi)$ is as in equation (6), and the general storage term is given by (4).

The method used to evaluate the derivative term in σ, and the derivatives of k_{rw} and σ needed in the Newton scheme Jacobian, may affect the convergence behavior of the iterative schemes. Numerical differentiation is often used to prevent floating point overflow near singularities, or to avoid oscillations around points of inflection. Parameter KSLOPE in the FLOW3D code offers five options for analytical or numerical differentiation of the characteristic equations, including purely analytical differentiation, a tangent slope formula, and the chord slope approximation suggested by Huyakorn *et al.* [4].

In addition to the parameters associated with the soil constitutive relations, the FLOW3D code requires input of the saturated hydraulic conductivity tensor k_{ij}, the porosity n, and the specific storage S_s. The saturated conductivity values along the x, y, and z coordinate directions are stored in arrays PERMX, PERMY, and PERMZ, the porosity values in POROS, and the elastic storage values in ELSTOR. To handle spatial heterogeneity, the porous medium is subdivided into NZONE regions in the horizontal plane and NSTR vertical layers, and one value of the material properties PERMX, PERMY, PERMZ, POROS, and ELSTOR is input for each of these regions and layers.

3-D Mesh and Boundary and Initial Conditions

Mesh generation for the FLOW3D code is the same as for the LEA3D and NON-LEA3D transport codes, and is described in the companion paper.

The FLOW3D model handles several types of complex time-varying boundary conditions, which are specified in three separate input files. The first input file is for atmospheric boundary conditions, which consist of homogeneous or spatially distributed rainfall (positive) and/or evaporation (negative) fluxes at the surface. The input flux values are considered "potential" rainfall or evaporation rates, and the actual rates, which depend on the prevailing flux and pressure head values at the surface, are dynamically calculated by the code during the simulation. A surface node can therefore switch from a specified flux (Neumann) to a constant head (Dirichlet) boundary condition, and vice versa, during the course of a simulation. This special treatment of atmospheric fluxes is described in Paniconi and Wood [5].

The second input file is for seepage faces, which can be placed, for example, along a pumping well, landfill ditch, or streambank. Like atmospheric boundary conditions, seepage faces also require special treatment. The method used in the FLOW3D code is a variant of the procedure described by Cooley [6], whereby the code automatically updates the position of the seepage face exit point after every iteration and time step. The nodes above the exit point are treated as zero flux Neumann boundary conditions, and those below as zero pressure head Dirichlet conditions. The code provides two parameters, ISFONE and ISFCVG, which can be used to relax the convergence requirement for the solution along seepage faces.

The third input file is for standard, non-switching Neumann and Dirichlet boundary conditions. These can be used to simulate, for example, the discharge or recharge rates at a pumping well, or the hydrostatic conditions along a stream. The parameters HTIDIR and HTINEU specify whether the boundary conditions are time-varying or constant.

Initial conditions can be read in as a single pressure head value which is replicated to all nodes (INDP = 0), or they can be input nonuniformly, one value for each node (INDP = 1).

Numerical Solution, Nonlinear Iteration, and Linear Solvers

The numerical solution of equation (1) is based on a finite element Galerkin discretization in space with linear basis functions, and a weighted finite difference scheme in time. The weighting parameter is TETAF, with a value of 1.0 giving a backward Euler scheme and a value of 0.5 corresponding to the Crank-Nicolson method. The code provides the option of using either distributed or lumped mass matrices (parameter LUMP). Details of the numerical procedures are given in Gambolati *et al.* [7].

The two most commonly used approaches for solving the nonlinear system of equations resulting from the numerical discretization of (1) are available in FLOW3D. Picard iteration (IOPT = 1) is simple and preserves symmetry of the finite element matrices, but may fail or converge slowly. Newton iteration (IOPT = 2) is more costly and yields nonsymmetric system matrices, but it can be more robust and faster-converging than the Picard method. Convergence of the Picard and Newton procedures can sometimes be enhanced by nonlinear relaxation, and FLOW3D provides the option of using either a constant relaxation parameter OMEGA (NLRELX = 1) or an iteration-dependent OMEGA (NLRELX = 2). More information on nonlinear iteration and relaxation is given in Paniconi and Putti [8]. Since Newton iteration produces a nonsymmetric system while the Picard method preserves symmetry, different solvers are used for the resulting linear systems. These are described in the companion paper.

Dynamic Time Stepping and Model Outputs

Time step sizes during a transient simulation are dynamically adjusted according to the convergence behavior of the nonlinear iteration scheme. A convergence tolerance TOLUNS is specified, along with a maximum number of iterations, ITUNS, permitted during any time step. The simulation begins with a time step size of DELTAT and proceeds until time TMAX. The current time step size is increased to DELTAT × DTMAGM + DTMAGA (to a maximum size of DTMAX) if convergence is achieved in fewer than ITUNS1 iterations, it is left unchanged if convergence required between ITUNS1 and ITUNS2 iterations, and it is decreased to DELTAT × DTREDM − DTREDS (to a minimum of DTMIN) if convergence required more than ITUNS2 iterations. If convergence is not achieved (ITUNS exceeded), the solution at the current time level is recomputed ("back stepping") using a reduced time step size (DELTAT × DTREDM − DTREDS). For the first time step of a transient simulation, or for steady state problems, the initial conditions are used as the first solution estimate for the iterative procedure. For subsequent time steps of a transient simulation, the pressure head solution from the previous step is used as the first estimate.

Output from the FLOW3D code includes:

- Mirroring of all the input data, as well as information about the three-dimensional mesh which has been generated;
- Information at each time step about the convergence behavior of the linear solver and nonlinear iterative scheme;
- Information at each time step about the mass balance errors;
- Pressure head, water saturation, and relative conductivity values at user-selected nodes at each time step;
- Detailed output at the start and end of the simulation, and at user-selected interim time values, of: pressure head, velocity, water saturation, and relative conductivity at all nodes; velocity and water saturation on all elements; vertical profiles of pressure head, water saturation, and relative conductivity at user-selected surface nodes; pressure head and water saturation at the surface nodes, along with a saturation index indicating whether the node is unsaturated, or saturated due to either the infiltration excess (Horton) mechanism or the saturation excess (Dunne) mechanism (Paniconi and Wood [5]);
- Hydrographs showing the atmospheric, seepage, overland (runoff), and subsurface fluxes at each time step.

The detailed output of water saturation and velocity values can be used as input to the LEA3D and NONLEA3D transport codes, which are described in a companion paper.

Numerical Example

To illustrate the use and features of the FLOW3D code, we present a numerical example of flow and transport in a ditch-drained aquifer with incident steady rainfall and trickle infiltration of a contaminant. The test case was described by Gureghian [9], modified by Gambolati *et al.* [7], and is further extended here to include two low-permeability clay lenses in the unconfined aquifer and to consider both two-dimensional and three-dimensional scenarios.

Figure 1 is a sketch of the test problem showing various possible configurations: homogeneous or heterogeneous cases can be simulated by assigning different material or hydraulic properties to the clay lenses; two or three-dimensional flow and transport patterns can be obtained by considering either the rectangular strip or the circular area as the contaminant source at the surface. In the results presented here and in the companion paper we ignore the clay lenses and assume trickle infiltration from the circular area. A Darcy flux

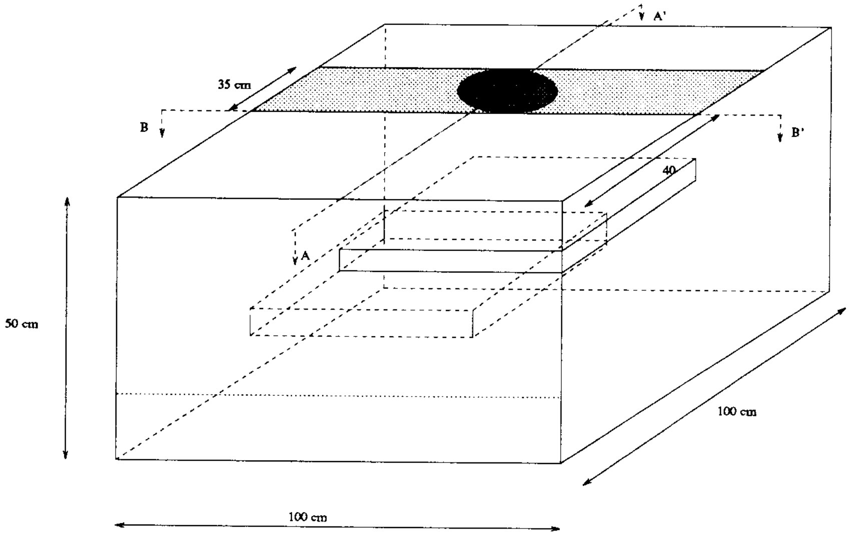

Figure 1: Sketch of the example problem.

$(v_i = -k_{ij}k_{rw}(\partial\psi/\partial x_j + \zeta_j))$ of 0.15 cm/d is applied over the circular area, while the rest of the surface is subjected to a Darcy flux of 0.1 cm/d. A seepage face boundary condition is applied along the front vertical face (parallel to section BB$'$, at A). Boundary conditions of zero Darcy flux are imposed along the other three vertical faces, and at the base of the aquifer. The aquifer system is isotropic and homogeneous, with a saturated hydraulic conductivity of 40 cm/d and a porosity of 0.3. Equations (6) and (8) describe the soil hydraulic properties, with $\epsilon = 0.015$, $\eta = 2$, $\gamma = 3$, $\psi_a = -10$ cm, $S_{wr} = 0.01$, $a = 2$, and $b = 3.5$.

The domain contains 2009 nodes and 3840 triangles at the surface, and is discretized into 20 vertical layers, to yield 42189 nodes and 230400 tetrahedra for the 3-D grid. The simulation was run in steady state, and the resulting pressure head contours and velocity field along cross section AA$'$ are shown in Figure 2.

Conclusions

FLOW3D is an efficient and flexible finite element code for the simulation of realistic saturated and unsaturated flow problems, both for stand-alone groundwater studies or to generate the velocity and water saturation distributions needed for the LEA3D and NONLEA3D reactive transport codes.

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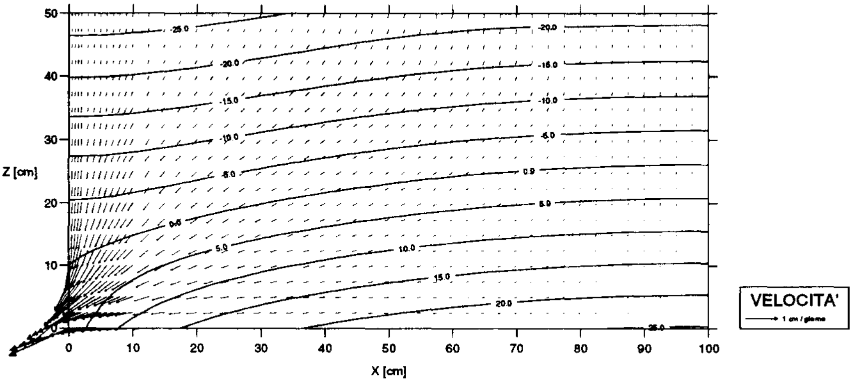

Figure 2: Steady state pressure head contours and velocity field for the example problem.

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