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Mixed Hybrid Finite Element formulation for water flow in unsaturated porous media

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Abstract

The Mixed Hybrid Finite Element formulation is applied to the simulation of water flow in unsaturated porous media, especially in clayey media. Two phases are taken into account: water and air. Air is compressible and soluble. The infiltration model is solved numerically using capillary and air head pressures as main variables. The use of head pressures prevents stability problems induced by gravity. The time discretization is fully implicit and the equations are solved within a sequential iterative Picard scheme. The hybridization of the formulation enables the homogeneization of non linear parameters on each mesh and leads to a better precision. Several validation and qualification tests, of increasing complexity, are presented.

1 Introduction

In most of the studies on water infiltration in a porous medium, air phase can be ignored, since this phase is assumed to be connected with the atmosphere. However this is not the case when modeling saturation processes in a high level waste deep geological repository. As a matter of fact, in such a repository, clayey buffer materials should be disposed around wastes, in shafts and galeries. After closure it is expected that water of the host rock will saturate these buffer materials and air will be trapped. Moreover, due to thermal gradients created by waste, vapour should be taken into account. The model describing these processes [1] is basically the model of mass transport of multiple fluid phases [2]. Most of the codes devoted to this problem are based on a Galerkin finite element formulation. It is recognized that this formulation presents some drawbacks as, for example, the non respect of mass conservation [3]. We present here an application of the mixed hybrid finite element formulation [3] to the problem. The mixed feature of the formulation enables to solve simultaneously Darcy and mass balance equations for each phase and the hybrid feature enables an accurate approximation on each mesh of the non linear parameters.

This formulation has been implemented in the finite element code CASTEM2000 [4, 5]. Several validation tests, of increasing complexity, are presented. In the first one, water is the only phase. In the second, air is assumed to be incompressible. Finally air compressibility and solubility are taken into account.

2 Physical Model

Water infiltration in an unsaturated clayey material is governed by the transport of three phases: water, dry air and vapour [1]. The mass balance equation for water, assumed to be incompressible, is

$$\frac{\partial \theta_W}{\partial t} + \vec{\nabla}.\vec{U}_W = 0 \tag{1}$$

The mass balance for total air (air and dissolved air):

$$\frac{\partial(\rho_A(\theta_A + H_C\theta_W))}{\partial t} + \vec{\nabla}.\left(\rho_A\left(\vec{U}_A + H_C\vec{U}_W\right)\right) = 0 \tag{2}$$

where dissolved air, of density $H_C\,\rho_A$, is advected by water. θ_α and ρ_α are respectively the volumetric content and the mass density of phase α ($\alpha = W(\text{water}), A(\text{air})$); H_C is Henry's constant and $\vec{U}_\alpha$ is the generalized Darcy velocity defined as

$$\vec{U}_\alpha = -\frac{k_\alpha}{\mu_\alpha}(\vec{\nabla}P_\alpha - \rho_\alpha\vec{g}) \tag{3}$$

where k_α and μ_α are respectively the effective permeability and the dynamic viscosity of phase α; P_α is the pressure and $\vec{g}$ the vector of gravity acceleration.

Vapour comes from water evaporation and its transport is governed by two mechanisms: advection by air and Fick diffusion, due to vapour concentration gradient. In an isothermal system, which is the case dealt here, vapour can be neglected in a first approximation.

The system of equations is completed with the three following state equations: the saturation equality $\omega = \theta_A + \theta_W$, the capillary pressure law $P_C(\theta_W) = P_A - P_W$, the law of perfect gas $P_A = \rho_A RT$ where R is the perfect gas constant. The model is solved in terms of two primary variables, the air head pressure, $h_A = (P_A - P_0)/\rho_W g$, and the capillary head pressure, $h_C = -(P_C - P_0)/\rho_W g = h_W - h_A$, where P_0 is the atmospheric pressure and h_W is the water head pressure. The equations to be solved are finally:

$$C(h_C)\frac{\partial h_C}{\partial t} = \vec{\nabla}.\left(K_W(\theta_W)\left(\vec{\nabla}h_A + \vec{\nabla}h_C + \vec{\nabla}z\right)\right) \tag{4}$$

$$(\omega - \theta_W + H_C\theta_W)\frac{\partial h_A}{\partial t} - \rho_A(1 - H_C)C(h_C)\frac{\partial h_C}{\partial t} = \tag{5}$$
$$\vec{\nabla}.\left(\left(\rho_A K_A(\theta_W) + \rho_A H_C K_W(\theta_W)\right)\vec{\nabla}h_A\right) + \vec{\nabla}.\left(\rho_A H_C K_W(\theta_W)\left(\vec{\nabla}h_C + \vec{\nabla}z\right)\right)$$

where C is the capillary capacity and K_α the unsaturated hydraulic conductivity, or unsaturated permeability, of phase α.

3 Numerical Resolution

For the sake of clarity we show in a first step how Richard's equation is solved with a mixed hybrid finite element formulation.

3.1 Richard's equation

Neglecting the air phase the equations to be solved are

$$\begin{cases} C(h)\dfrac{\partial h}{\partial t} = -\vec{\nabla}.\vec{U} \\ \vec{U} = -K(\theta)(\vec{\nabla}h + \vec{\nabla}z) \end{cases} \tag{6}$$

The time discretization is fully implicit and the nonlinear terms are solved within a Picard algorithm:

$$\begin{cases} C^{N+1,I} \dfrac{H^{N+1,I+1} - H^{N}}{\Delta t} = -\vec{\nabla}.\vec{U}^{N+1,I+1} \\ \vec{U}^{N+1,I+1} = -K^{N+1,I}\vec{\nabla}H^{N+1,I+1} \end{cases} \tag{7}$$

where H=h+z, N stands for the time discretization and I for the Picard 's iteration. This algorithm allows to keep the parabolic form of the problem, i.e. no advective term due to gravity appears. Within a mixed hybrid finite element formulation, the variational formulation of eqn (6) gives for an element Ω [4]:

$$\begin{cases} \int_{\Omega} K^{-1}\vec{U}.\vec{w}\, d\Omega = \int_{\Omega} h\vec{\nabla}.\vec{w}\, d\Omega - \int_{\Omega} h\vec{w}.\vec{n}\, d\Gamma \\ \int_{\Omega} C(h)\dfrac{\partial h}{\partial t} v\, d\Omega = -\int_{\Omega} \vec{\nabla}.\vec{U} v\, d\Omega \end{cases} \tag{8}$$

where $\vec{w}$ and v are basis functions. The variables appearing in these integrals are: the mean velocity across a face, the mean head on a face, called head trace, and the mean head in an element. In order to compute these integrals one must define on the element mean values of capillary capacity and inverse of hydraulic conductivity. The natural choice would be to take the values of these parameters for the mean head. Hybridization allows others choices. Our experience shows that the best one, in term of precision, is the arithmetic mean of the parameter traces on an element (the parameter trace is the parameter value for the head trace).

3.2 General model

In order to solve eqns (4) and (5) within a mixed hybrid finite element formulation we rewrite them under the following generic form:

$$\begin{cases} A_{1,1} \dfrac{\partial h_C}{\partial t} = -\vec{\nabla}.(\vec{U}_{1,1} + \vec{U}_{1,2}) \\ A_{2,1} \dfrac{\partial h_C}{\partial t} + A_{2,2} \dfrac{\partial h_A}{\partial t} = -\vec{\nabla}.(\vec{U}_{2,1} + \vec{U}_{2,2}) \end{cases} \tag{9}$$

where the A coefficients depend on h_C and h_A. $\vec{U}_{1,1}$ and $\vec{U}_{2,1}$ are proportional to $\vec{\nabla}h_C + \vec{\nabla}z$; $\vec{U}_{1,2}$ and $\vec{U}_{2,2}$ are proportional to $\vec{\nabla}h_A$. We use again a fully implicit scheme and the equations are solved within a sequential Picard iterative algorithm:

$$\begin{cases} A_{1,1}^{N+1,I} \dfrac{h_C^{N+1,I+1} - h_C^N}{\Delta t} + \vec{\nabla}.\vec{U}_{1,1}^{N+1,I+1} = -\vec{\nabla}.\vec{U}_{1,2}^{N+1,I} \\ A_{2,2}^{N+1,I} \dfrac{h_A^{N+1,I+1} - h_A^N}{\Delta t} + \vec{\nabla}.\vec{U}_{2,2}^{N+1,I+1} = -\vec{\nabla}.\vec{U}_{2,1}^{N+1,I+1} - A_{2,1}^{N+1,I} \dfrac{h_C^{N+1,I+1} - h_C^N}{\Delta t} \end{cases} \quad (10)$$

The righthand terms of these equations are treated as source terms. $\vec{U}_{1,2}$ and $\vec{U}_{2,1}$ are computed through the proportionality relationships: $\vec{U}_{1,2} = \alpha\vec{U}_{2,2}$ and $\vec{U}_{2,1} = \beta\vec{U}_{1,1}$. Due to hybridization, α and β coefficients are defined on the faces of an element and, consequently, these relationships make sense. Let us point out that this algorithm is mass conservative, but demonstration will not be given here. The variational formulation can be easily applied to these equations.

4 Validation-Application

This algorithm has been implemented in the finite element code CASTEM2000, which is a general computational tool developed at the CEA for mechanics and fluid mechanics applications [4, 5]. It has been validated and tested on several 1D, 2D and 3D cases reported in the literature. We present three 1D validation test cases.

4.1 Vertical infiltration in Yolo light clay

Vauclin [6] proposed, for the Yolo light clay, a closed form of Philip's solution to the 1D vertical infiltration problem. The unsaturated permeability is $K(h) = K_S \dfrac{A}{A + |h|^B}$ and the water retention curve: $\theta(h) = \theta_R + \dfrac{\alpha(\omega - \theta_R)}{\alpha + (\ln|h|)^\beta}$ for $-700\,\text{cm} \le h < -1\,\text{cm}$ and $\theta = \omega$ for $h \ge 1\,\text{cm}$,

where K_S is the saturated permeability, h is the head pressure and θ_R the residual water content. Values of the parameters are given in [6].

The vertical dimension of the domain is 1 meter with $\Delta z = 1\,\text{cm}$. A water pressure equal to zero is applied at the top of the domain. Figure 1 shows the numerical and Vauclin's water content profiles at different times. The agreement is good, nevertheless, at long times, there is a slight delay between the two profiles. This is probably due to the first order time discretization scheme. The time step is approximatively constant and equal to one hour. After a few time steps, convergence is achieved in four iterations for a tolerance criterion on water content of 10^{-5}.

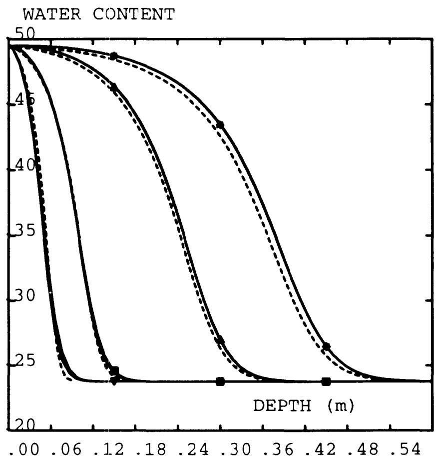

Figure 1: Vertical infiltration in a Yolo light clay ; Water content at different times (Full line : numerical results, Dashed line : Philip's solutions)

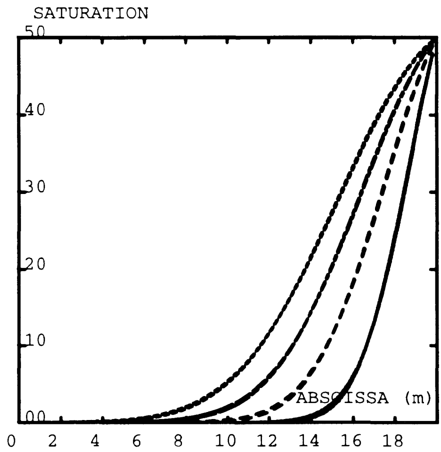

Figure 2: Two phase flow analytical case; Numerical and analytical phase 1 content profiles at different times (The two profiles are merged.)

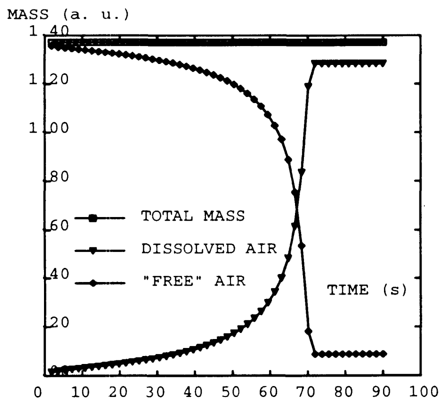

Figure 3: Air-water flow. Air mass as a function of time.

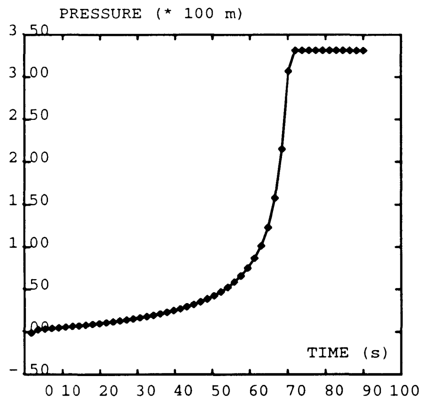

Figure 4: Air-water flow. Air pressure as a function of time.

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4.2 Two-phase flow analytical case

This test case has been studied by François [7]. It has no physical significance but is close to a two-phase flow problem where one phase is pushing the other one. The two phases are immiscible and incompressible. The interest of this test case is that phase one content obeys to a classical diffusion advection equation and therefore is easy to compute analytically. The unsaturated permeabilities of the two phases are linear: $K_1(\theta_1) = \theta_1$, $K_2(\theta_1) = 1 - \theta_1$. Water retention curve is $h_C(\theta_1) = k \log \frac{\theta_1}{1 - \theta_1}$. Initial conditions are $\theta_1(x,0) = 0$, $h_2(x,0) = 0$, and the boundary conditions are $\theta_1(L,t) = 0.5$ and $h_2(L,t) = 0$, $\theta_1(0,t) = 0$ and $\vec{\nabla} h_2(0,t).\vec{n} = +1$. The domain extent is L=20 meters with $\Delta x = 0.4\,\mathrm{m}$. The numerical and analytical profiles of phase one content are plotted on figure 2 at different times for k = 2. The agreement is good. The phase two pressure profile is quasi linear and quasi constant in time.

4.3 Air-water flow

This test case describes water infiltration in a column of sand filled initialy with air and with zero air flow boundary conditions. Consequently air is compressed and dissolved in water. One of the objective of this test case is to verify the air mass conservation in the system [1]. The unsaturated permeabilities of water and air are respectively $\mathrm{Log}_{10}(K_W(\theta_W)) = A + B\theta_W + C/\theta_W$ and $K_A(\theta_W) = K_{AS} \frac{\theta_S - \theta_W}{\theta_S - \theta_R}$ where K_{AS} is the air saturated permeability. The water retention curve is $\theta_W(h_C) = \frac{A + h_C}{-C - Bh_C}$. The values of the different parameters are given in [1]. The initial conditions in the column are: air pressure equal to 100 KPa and residual water content of 10%. All boundaries are impervious to air and water except the top of the column where a head pressure of 2 meters is imposed. The length of the column is 0.026 m. and $\Delta z = 10^{-3}\,\mathrm{m}$. The time step is approximatively constant and equal to 0.2 seconds. Figure 3 gives the dissolved, non dissolved and total air mass in the column as a function of time. We see that total air mass is conserved. As the infiltration front moves downwards the volume of air decreases and air pressure increases. Figure 4 shows the evolution with time of air pressure. Let us note that this pressure is approximatively constant in space.

5 Conclusion

Other validation test cases have been studied such as vertical infiltration in a heterogeneous soil or hydratation of a cylindrical clay engineered barrier. At the present time the model is coupled in CASTEM2000 to a finite element model describing the mechanical comportment of a swelling clay material. Within the framework of the European project RESEAL this coupling is used to model the hydro-mechanical comportment of a clay plug. Concerning the future developments it is planned to take into account the vapour phase and to couple the model to an energy balance equation. This will permit to study the full thermo-hydro-mechanical coupling in a clayey buffer material of a high level waste repository.

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