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Original article

Gas phase appearance and disappearance as a problem with complementarity constraints☆

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Abstract

The modeling of migration of hydrogen produced by the corrosion of the nuclear waste packages in an underground storage including the dissolution of hydrogen involves a set of nonlinear partial differential equations with nonlinear complementarity constraints. This article shows how to apply a modern and efficient solution strategy, the Newton-min method, to this geoscience problem and investigates its applicability and efficiency. In particular, numerical experiments show that the Newton-min method is quadratically convergent for this problem.

Keywords: Porous media; Two-phase flow; Nuclear waste underground storage; Nonlinear complementarity problem; Newton-min

1. Introduction

The Couplex-Gas benchmark [22] was proposed by Andra (French National Inventory of Radioactive Materials and Waste) [3] and the research group MoMaS (Mathematical Modeling and Numerical Simulation for Nuclear Waste Management Problems) [21] in order to improve the simulation of the migration of hydrogen produced by the corrosion of nuclear waste packages in an underground storage. This is a system of two-phase (liquid–gas) flow with two components (hydrogen–water). The benchmark generated some interest and engineers encountered difficulties in handling the appearance and disappearance of the phases. The resulting formulation [15] is a set of partial differential equations with nonlinear complementarity constraints. Even though they appear in several problems of flow and transport in porous media like the black oil model presented in [8] or transport problems with dissolution–precipitation [7,17,19], complementarity problems are not usually identified as such in hydrogeology and, to circumvent the solution of complementarity conditions, problems are often solved by reformulating the problem as in [1,2,6]. However the solution of complementarity problems is an active field in optimization [5,10,13] and we draw from the know-how of this scientific community. A similar path is followed bin papers like [12,18,20]. The application of a semi-smooth Newton method [14,16], sometimes called the Newton-min algorithm, to solve nonlinear complementarity problem is

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described. We will demonstrate through a test case, the ability of our model and our solver to efficiently cope with appearance or/and disappearance of one phase.

In Section 2, we introduce the formulation of the problem and in Section 3 we describe the numerical method. In Section 4, we present and discuss a numerical experiment.

2. Problem formulation

This section gives a precise formulation of the mathematical model for the application that was outlined in the introduction. We consider a problem where the gas phase can disappear while the liquid phase is always present.

2.1. Fluid phases

Let ℓ and g be the respective indices for the liquid phase and the gas phase. Darcy's law reads

$$\mathbf{q}_i = -K(x)k_i(s_i)(\nabla p_i - \rho_i g \nabla z), \quad i = \ell, g, \tag{1}$$

where K is the absolute permeability. For each phase $i = \ell, g$, s_i is the saturation and $k_i = k_{ri}(s_i)/\mu_i$ is the mobility with k_{ri} the relative permeability and μ_i the viscosity (assumed to be constant). The mobility k_i is an increasing function of s_i such that $k_i(0) = 0$, $i = \ell, g$. Assuming that the phases occupy the whole pore space, the phase saturations satisfy

$$0 \le s_i \le 1, \quad s_\ell + s_g = 1.$$

The phase pressures are related through the capillary pressure law

$$p_c(s_\ell) = p_g - p_\ell \ge 0,$$

assuming that the gas phase is the non-wetting phase. The capillary pressure is a decreasing function of the saturation s_ℓ.

In the following, we will choose s_ℓ and p_ℓ as the main variables since we assume that the liquid phase cannot disappear for the problem under consideration.

2.2. Fluid components

We consider two components, water and hydrogen, identified by the indices $j = w, h$. The mass density of the phase is

$$\rho_i = \rho_w^i + \rho_h^i, \quad i = \ell, g.$$

From M^w and M^h, the water and hydrogen molar masses, we define the molar concentration of phase i:

$$c_i = c_w^i + c_h^i, \quad c_j^i = \frac{s_i \rho_j^i}{M^j}, \quad j = w, h, \quad i = \ell, g. \tag{2}$$

The molar fractions are

$$\chi_h^i = \frac{c_h^i}{c_i}, \quad \chi_w^i = \frac{c_w^i}{c_i}, \quad i = \ell, g. \tag{3}$$

Obviously,

$$\chi_w^i + \chi_h^i = 1, \quad i = \ell, g. \tag{4}$$

We assume that the liquid phase may contain both components, while the gas phase contains only hydrogen, that is the water does not vaporize. In this situation we have

$$\rho_w^g = 0, \quad \rho_g = \rho_h^g, \quad \chi_h^g = \frac{c_h^g}{c_g} = 1, \quad \chi_w^g = 0.$$