Abstract
In a two-phase (liquid–gas) two-component (water–hydrogen) system we discuss the formulation of the possible dissolution of hydrogen in the liquid phase. We show how Henry’s law fits in a phase diagram and the problem is formulated as a set of nonlinear partial differential equations with complementarity constraints.

Keywords
Two-phase flow · Porous media · Dissolution · Henry’s law · Nuclear waste underground storage · Complementarity constraints

1 Introduction
Recently, the Couplex-Gas benchmark (http://www.gdrmomas.org/ex_qualifications.html) was proposed by Andra and MoMAS 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). This is similar to a black-oil model. The benchmark requires to use Henry’s law to model the dissolution of hydrogen. This benchmark generated some interest and engineers encountered difficulties in handling the appearance and disappearance of the phases. Recently, two other papers Bourgeat et al. (2009), Abadpour and Panfilov (2009) addressed the formulation of this problem.
In this article, for the sake of simplicity of exposition, we assume that only hydrogen is in the gas phase (water does not vaporize). We discuss how to extend Henry’s law to the case where the gas phase disappears. This is done by showing how Henry’s law fits in a phase diagram. The resulting formulation is a set of partial differential equations with complementarity constraints. A similar formulation is also presented in Bourgeat et al. (2009) and it can also be viewed as a variation of the formulation of the black oil model presented in Chavent and Jaffré (1986).

2 Mathematical Formulation

We first describe the equations and some simplifying hypotheses. Since we consider a problem where the gas phase can disappear while the liquid phase cannot disappear, we will consider a formulation using the saturation and the pressure of the liquid phase as the two main unknowns.

2.1 Fluid Phases

ℓ and g are the respective indices for the liquid phase and the gas phase. Darcy’s law reads

\[ q_i = -K(x)k_i(s_i)(\nabla p_i - \rho_i \rho g \nabla z), \quad i = \ell, g, \]  

(2.1)

where \( K \) is the absolute permeability. Assuming that the phases occupy the whole pore space, the phase saturations \( s_i, i = \ell, g \) satisfy

\[ 0 \leq s_i \leq 1, \quad s_\ell + s_g = 1. \]

The mobilities are denoted by \( k_i(s_i) = \frac{k_{ri}(s_i)}{\mu_i} \) with \( k_{ri} \) the relative permeability, and \( \mu_i \) the viscosity of the phase \( i = \ell, g \), assumed to be constant. The mobility \( k_i \) is an increasing function of \( s_i \) such that \( k_i(0) = 0, i = \ell, g \).

The phase pressures are related through the capillary pressure law

\[ p_c(s_\ell) = p_g - p_\ell \geq 0 \]

(2.2)

assuming that the gas phase is the nonwetting phase. The capillary pressure is a decreasing function of the saturation \( s_\ell \) such that \( p_c(1) = 0 \).

In the following, we choose \( s_\ell, p_\ell \) 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, denoted by the indices \( j = w, h \). The mass density of the phase \( i \) is

\[ \rho_i = \rho^i_w + \rho^i_h, \quad i = \ell, g, \]

where \( \rho^i_w \) and \( \rho^i_h \) are the mass concentrations of water and hydrogen in the phase \( i, i = \ell, g \), respectively. The mass fractions are

\[ \chi^i_h = \frac{\rho^i_h}{\rho_i}, \quad \chi^i_w = \frac{\rho^i_w}{\rho_i}, \quad i = \ell, g. \]