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A coupled hydro-mechanical model for simulation of gas migration in host sedimentary rocks for nuclear waste repositories

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ABSTRACT

In a deep geological repository (DGR) for nuclear wastes, several mechanisms such as waste form degradation and corrosion could lead to gas generation. The produced gas can potentially overpressurize the repository, alter the hydraulic and mechanical properties of the host rock and affect the long term containment function of the natural (host rock) and engineered barriers. Thus, the understanding of the gas migration within the host rock and engineered barriers and the associated potential impacts on their integrity is important for the safety assessment of a DGR. In this paper, a coupled hydro-mechanical model for predicting and simulating the gas migration in sedimentary host rock is presented. A detailed formulation coupling moisture (liquid water and water vapor) and gas transfer in a deformable porous medium is given. The model takes into account the damage-controlled fluid (gas, water) flow as well as the coupling of hydraulic and mechanical processes (e.g., stress, deformation). The model also considers the coupling of the diffusion coefficient with mechanical deformation as well as considers the modification of capillary pressure due to the variation of permeability and porosity. The prediction capability of the developed model is tested against laboratory scale and in situ experiments conducted on potential host sedimentary rocks for nuclear waste disposal. The model predictions are in good agreement with the experimental results. The numerical simulations of the laboratory and field gas injection tests provide a better understanding of the mechanisms of gas migration and the potential effects of excessive gas pressure on the host sedimentary rocks. This research work has allowed us to identify key features related to gas generation and migration that are considered important in the long term safety assessment of a DGR in sedimentary host formations.

1. Introduction

The disposal of nuclear waste in deep sedimentary rock formations is currently investigated in several countries (e.g., Canada, France, Germany, India, Switzerland). For example, in Canada, a repository for low and intermediate level radioactive wastes is being proposed in Ontario's sedimentary rock formations (Nasir et al., 2011, 2013; Fall and Nasir, 2011). Significant quantities of gas can be generated in underground repositories for radioactive waste. The main mechanisms of gas generation in an underground nuclear waste repository are corrosion of metals in waste containers and/or in the waste, radiolysis of water and organic materials and microbial degradation of organic materials. The gas generation rates are likely to be significantly higher for repositories with intermediate level waste (ILW) and low level waste (LLW) than for those with high level waste (HLW) or spent fuel. The reason is that there are larger volumes of metals and organic materials in the former compared to the latter two (Rodwell, 1999) types of repositories. These gases could migrate through engineered and natural geological barrier systems. The pressure in the generated gas would build up, and could induce the formation of either microcracks or macrocracks and/or enlarge the pore structure of the barrier material. This could affect the long-term performance of the barriers against contaminant transport (Fig. 1). Furthermore, these gases could significantly impact the biosphere and groundwater as shown in Fig. 1. Thus, the assessment of the long term safety of a repository for nuclear waste in deep sedimentary rock formation requires a good understanding of the process of gas migration and its impact on the host rock.

The understanding of gas migration and its potential impact on the host sedimentary rocks has been a key target for all major international waste isolation programs (e.g., ANDRA in France, NDA in UK, NAGRA in Switzerland, NWMO in Canada, SKB in Sweden, SCK-CEN in Belgium). During the past years, main research efforts have been spent on gas migration in sedimentary rock. Several laboratory experiments on gas transport through natural (e.g., argillite) or engineered (e.g., bentonite) porous media have been performed (e.g., Horseman et al., 1999; Galle, 2000; Davy et al., 2007; Arnedo et al., 2008). These studies have shown that the migration of gas in porous media (e.g., sedimentary

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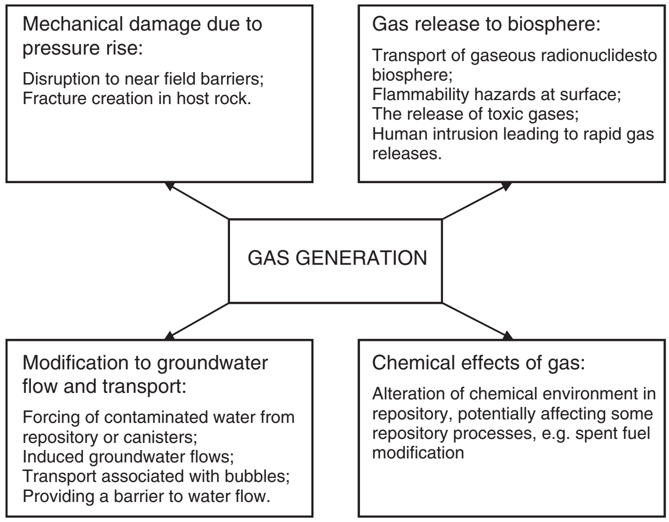

Fig. 1. Schematic of the range of effects that may follow from gas generation in a repository (Rodwell et al., 2003).

rock) is a complex phenomenon. Gas migration in porous media is governed by the coupling between several processes such as mechanical (e.g., stress, deformation, damage) and hydrological (e.g., flow of water, gas flow, pore fluid pressure, phase change) processes. At the time of writing however, only a few modeling studies (e.g., Lege and Shao, 1996; Ortiz et al., 1996; Alonso et al., 2006; Du et al., 2006; Gerard et al., 2008) were conducted to develop mathematical and/or numerical models that can capture the main physical processes associated with gas migration in sedimentary rocks, and are able to predict gas migration and its impacts on the host sedimentary rock. Furthermore, many of the previous modeling research (e.g., Ortiz et al., 1996; Gerard et al., 2008) didn't consider the interplay between hydraulic and mechanical processes (e.g., stress, deformation, dilatancy, damage) or mostly dealt with uncoupled processes (e.g., two phase flow). Modeling gas migration in host sedimentary rock requires the introduction of mathematical formulations that allow the consideration of coupled hydro-mechanical processes as mentioned above.

The objectives of the present paper are:

- To develop a fully coupled hydro-mechanical (HM) model for predicting the gas migration in initially unfractured sedimentary host rock. A hydro-poroelastic-damage model should be developed. The proposed mechanical model will be formulated within the framework of poroelasticity and continuum damage mechanics. Key features relevant for gas migration in host sedimentary rocks will be taken into account in the HM model, in particular the elastic degradation due to microcracks, coupling between permeability and induced damage, coupling between capillary pressure and induced damage, coupling between diffusion coefficient and induced damage, coupling between tortuosity and rock deformation and damage, influence of rock deformation on permeability, capillary pressure and diffusion coefficient, as well as variation of porosity with stress, deformation and induced damage;
- To verify the adequacy of the HM model against laboratory and in situ gas injection tests performed on a potential host sedimentary rock for nuclear;
- To model and simulate the key physical phenomena associated with gas migration in sedimentary rocks at laboratory and field experiment scale in order to better understand the mechanisms of gas migration in sedimentary rock and its effects on the rock integrity.

The paper will be organized as follows. The mathematical formulation of a coupled HM model of gas migration in damage-susceptible porous media is presented in the next section. This is followed by its verification and application in the simulation of gas injection laboratory and in situ experiments in Opalinus clay, from Mont Terri, Switzerland.

2. Mathematical formulation of the coupled hydro-mechanical model

2.1. Basis of the mathematical formulations and general assumptions

For modeling purposes of the porous medium (host sedimentary rock), we will adopt a continuum approach, in which a representative elementary volume (REV) around any mathematical point considered in the domain always contains both solid and fluid phases, and classical mass balance laws of continuum mechanics hold for each phase. The total volume of the medium is given by:

$$V = V_s + V_v \tag{1}$$

where V represents the total volume; V_s refers to the solid volume; and V_v refers to the void spaces occupied by the fluids (gas, liquid).

Since the porous medium is made of three phases (solid, s; liquid, l; and gas, g), it can be written that

$$V = V_s + V_l + V_g \tag{2}$$

$$M = M_s + M_l + M_g \tag{3}$$

where V_l, and V_g refer to the volumes of the liquid (water) and gas; and M, M_s, M_l and M_g are the total mass of the medium, the mass of the solid, liquid and gas, respectively.

The governing equations of the model result from a combination of a set of conservation and constitutive equations. The conservation equations include: (i) momentum and (ii) mass equations. The fundamental macroscopic conservation of an extensive thermodynamic property (e.g., mass, momentum) is applied here to derive those balance or conservation equations as described below. The macroscopic balance equation of any thermodynamic property in a continuum can be expressed in the following general form (Bear, 1972).

$$\frac{\partial}{\partial t} M_\pi^\kappa + \nabla \cdot (\mathbf{j}_\pi^\kappa) - f_\pi^\kappa = 0 \tag{4}$$

where the quantity M_π^κ can refer to the mass or energy per unit volume of the porous medium, with κ the mass components (air, water or solid) or "heat component", and π the phases (gas, liquid or solid). $\mathbf{j}_\pi^\kappa$ is the total flux (vector) with respect to a fixed reference system, and f_π^κ is the rate of the production/removal of component κ per unit volume.

To develop the governing equations, the following main assumptions are made:

(i) the porous medium includes three constituents: a solid and two fluids (water, gas). These constituents are considered as three independent overlapping continua in the context of the theory of mixtures (e.g., Goodman and Cowin, 1972; Morland, 1972; Atkin and Craine, 1976; Bowen, 1976, 1982; Hassanizadeh and Gray, 1979, 1980, 1990; Sampaio and Williams, 1979; Passman et al., 1984; Rajagopal and Tao, 1995). Water is a wetting fluid, whereas gas is not. The voids of the solid skeleton are partially filled with liquid water, and partially with gas;

(ii) the three constituents are distributed in the three phases as mentioned above. The gas phase is considered as an ideal gas mixture composed of dry air (gas generated by the repository is assumed to have the same properties as air and would be indistinguishable from it, ga index) and water vapor (gw index; it is entering the repository from the host rock). The vapor is transported within the gas phase by non-advective and advective fluxes.