Journal of Rock Mechanics and Geotechnical Engineering 6 (2014) 405–416

Contents lists available at ScienceDirect

Journal of Rock Mechanics and Geotechnical Engineering

journal homepage: www.rockgeotech.org

Full length article

Numerical analysis of thermal impact on hydro-mechanical properties of clay

Xuerui Wang [a,b,*], Hua Shao [a], Jürgen Hesser [a], Chunliang Zhang [c], Wenqing Wang [d], Olaf Kolditz [b,d]

[a] Federal Institute for Geosciences and Natural Resources – BGR, Hanover, Germany
[b] Technical University of Dresden, Dresden, Germany
[c] Gesellschaft für Anlagen- und Reaktorsicherheit – GRS, Braunschweig, Germany
[d] Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany

ARTICLE INFO

Article history:
Received 14 April 2014
Received in revised form
10 June 2014
Accepted 1 July 2014
Available online 7 August 2014

Keywords:
Radioactive waste disposal
Clayey rock
Heating experiment
Numerical modelling
OpenGeoSys (OGS)
Thermo-hydro-mechanical (THM) coupling
Multiphase flow
Thermal effect

ABSTRACT

As is known, high-level radioactive waste (HLW) is commonly heat-emitting. Heat output from HLW will dissipate through the surrounding rocks and induce complex thermo-hydro-mechanical-chemical (THMC) processes. In highly consolidated clayey rocks, thermal effects are particularly significant because of their very low permeability and water-saturated state. Thermal impact on the integrity of the geological barriers is of most importance with regard to the long-term safety of repositories. This study focuses on numerical analysis of thermal effects on hydro-mechanical properties of clayey rock using a coupled thermo-mechanical multiphase flow (TH^2M) model which is implemented in the finite element programme OpenGeoSys (OGS). The material properties of the numerical model are characterised by a transversal isotropic elastic model based on Hooke's law, a non-isothermal multiphase flow model based on van Genuchten function and Darcy's law, and a transversal isotropic heat transport model based on Fourier's law. In the numerical approaches, special attention has been paid to the thermal expansion of three different phases: gas, fluid and solid, which could induce changes in pore pressure and porosity. Furthermore, the strong swelling and shrinkage behaviours of clayey material are also considered in the present model. The model has been applied to simulate a laboratory heating experiment on claystone. The numerical model gives a satisfactory representation of the observed material behaviour in the laboratory experiment. The comparison of the calculated results with the laboratory findings verifies that the simulation with the present numerical model could provide a deeper understanding of the observed effects.

1. Introduction

Highly consolidated clay formations are investigated for deep geological disposal of heat-emitting high-level radioactive waste (HLW) due to their favourable properties such as extremely low hydraulic permeability, predominant diffusive mass transport, good isolation capability, homogeneous structure and especially high sorption capacity for most radionuclides, as well as the ability to seal cracks and fissures by swelling. However, heat output from HLW will dissipate through the surrounding rocks and induce complex thermo-hydro-mechanical-chemical (THMC) processes. Because of the very low permeability and the water-saturated state in clayey rocks, the thermal responses of clay formations are significant such as thermally induced pore pressure changes and therewith swelling and shrinkage behaviours, expansion and contraction due to temperature change, thermally induced deformation and change of strength. In order to investigate the thermal impact on clay host rocks, a large number of in situ heating experiments have been performed in underground research laboratories (URLs), i.e. the HE-D experiment on the Opalinus Clay in the Mont Terri Rock Laboratory in Switzerland (Wileveau, 2005; Zhang et al., 2009), the TER experiment on the Callovo-Oxfordian (COX) Clay at the Bure site in France (Wileveau and Su, 2007), and the ATLAS experiment on the Boom Clay in the rock laboratory Mol in Belgium (De Bruyn and Labat, 2002). Numerous in situ experiments have been carried out under defined conditions to estimate the material-specific parameters. However, there are still challenges to answer the following questions: What is the long-term thermo-hydro-mechanical (THM) behaviour of clay host rock in a realistic setting? Which possible changes of the material properties, such as

* Corresponding author. Tel.: +49 511 643 2953.
E-mail address: xuerui.wang@bgr.de (X. Wang).

Peer review under responsibility of Institute of Rock and Soil Mechanics, Chinese Academy of Sciences.

http://dx.doi.org/10.1016/j.jrmge.2014.07.002

permeability, porosity, stiffness and strength, could occur under the long-term heating and cooling processes? Is it necessary to consider the effects of gas thermal expansion, gas flow, and the phase change between gas and liquid in the pore space? What could be the consequences if micro-cracks or fractures formed? How could the integrity of the host rocks be affected by the long-term thermal impact?

The investigation of the above-mentioned issues requires a realistic numerical model which is calibrated by experimental data. This paper makes a contribution to describing the development of a coupled THM model to simulate the thermal influences on the hydro-mechanical processes. Generally, it is difficult to achieve a fully saturated state under natural or experimental conditions. Therefore, it is assumed that gas and water exist in the pore space at the same time. Both the gas and liquid phases could expand during heating; moreover, the liquid can be vaporised inside a gas-tight system. Thus, a multiphase flow model has been applied to describe the hydraulic processes for gas and liquid as well as the phase change. This model is based on associated theoretical formulations and the multiphase flow model in the finite element programme OpenGeoSys (OGS) (Kolditz et al., 2012a). According to the special properties of clay formations and the experimental conditions, some modifications have already been made in the OGS code. The developed numerical code has been applied to simulate a laboratory heating experiment on the Callovo-Oxfordian (COX) claystone which has been performed by GRS (Zhang et al., 2010). This modelling can reasonably reflect the observed responses of the claystone to the thermal loading.

2. Physical processes and numerical approaches

Generally, thermal effects can induce a complex interaction between THM processes. For instance (see Fig. 1), thermal loading can induce expansion of pore fluids and solid skeleton, and then change the pore space, leading to increase in pore pressure. Furthermore, the increase of temperature can cause a decrease in gas and liquid viscosity (T ≫ H). It can also induce a deformation with stress variations (T ≫ M). On the other hand, the change of pore pressure has an effect on the effective stress (H ≫ M) and the degree of water saturation. The water/gas flow can influence the heat conductivity (H ≫ T) because of the saturation-dependent thermal conductivity (Gens et al., 2007; Ghabezloo, 2010; Zhang et al., 2010). All the above-mentioned couplings have been considered in our numerical modelling.

To analyse the THM coupling processes, the porous medium is usually assumed as a homogenous continuum (Fig. 2). Generally, such porous media are composed of three species: mineral, water and gas, distributed as three phases: solid, liquid and gas (Kolditz et al., 2012b). The fluid phase contains water and dissolved air,

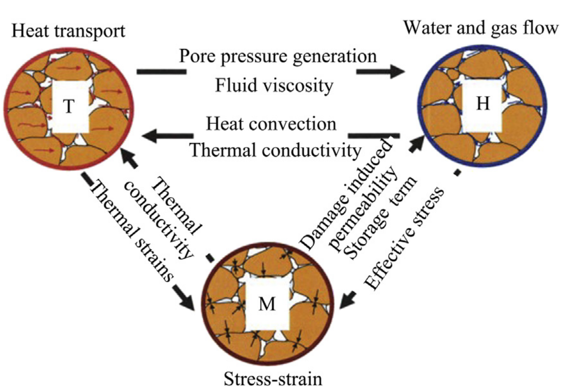

Fig. 1. Interactions between THM processes in porous media (Zhang et al., 2010).

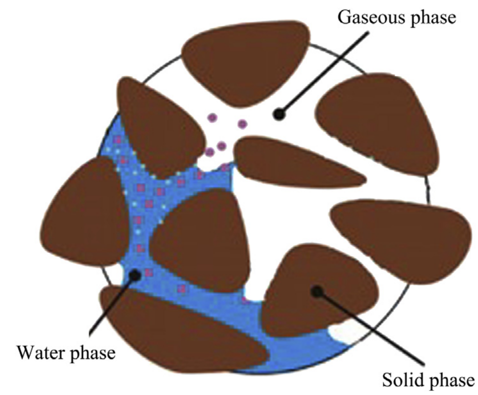

Fig. 2. Porous system with two-phase flow (Kolditz et al., 2012b).

while the gas phase is a mixture of dry air and water vapour. To present the behaviour of all three phases, a multiphase flow model is required for numerical analysis.

2.1. Balance equations

Mathematical descriptions of the physical coupled THM processes for saturated porous media have been proposed by several researchers (e.g. Booker and Savvidou, 1985; Olivella et al., 1994). Generally, for the solution of a coupled THM problem, a set of balance equations for internal energy, solid (s) mass, water (w) mass, gas (g) mass, and stress equilibrium have to be solved.

(1) Solid mass balance:

$$\frac{\partial}{\partial t}[\rho_s(1-\phi)] + \nabla \vec{J}_s = q_s \tag{1}$$

(2) Water mass balance:

$$\frac{\partial}{\partial t}(\rho_w S_w \phi) + \nabla \vec{J}_w = q_w \tag{2}$$

(3) Gas mass balance:

$$\frac{\partial}{\partial t}\left[\phi \rho_g (1-S_w)\right] + \nabla \vec{J}_g = q_g \tag{3}$$

(4) Internal energy balance:

$$\frac{\partial}{\partial t}\left[E_s\rho_s(1-\phi) + E_w\rho_w S_w\phi + E_g\rho_g(1-S_w)\phi\right] + \nabla\left(i_c + \vec{J}_{Es} + \vec{J}_{Ew} + \vec{J}_{Eg}\right) = q_E \tag{4}$$

(5) Stress equilibrium:

$$\nabla \boldsymbol{\sigma} + \boldsymbol{b} = \boldsymbol{0} \tag{5}$$

In Eqs. (1)–(5), ρ is the density; ϕ is the porosity; $\vec{J}$ is the total mass flux; q is the external mass supply per unit volume of medium; S_w is the degree of water saturation; E is the specific internal energy; i_c is the conductive heat flux; J_E is the energy flux due to mass motion; $\boldsymbol{\sigma}$ is the total stress tensor; $\boldsymbol{b}$ is the body forces vector; and subscripts “s”, “w”, and “g” stand for the solid, liquid and gas phases, respectively.