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A simulator for modeling of porosity and permeability changes in near field sedimentary host rocks for nuclear waste under climate change influences

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ABSTRACT

A new simulation tool is developed to model coupled thermo-hydro-mechanical-geochemical (THM-GeoC) processes that would occur in the near field of deep geological repositories (DGRs) for nuclear wastes, and their impacts on the evolution of the rock porosity and permeability. First, a coupled thermo-hydro-mechanical-chemical (THMC) model, in which, the chemical (C) process is limited to solute transport, is developed and then implemented into COMSOL Multiphysics finite element code. Then, two types of numerical software are coupled; the first is COMSOL Multiphysics code and the second is the PHREEQC geochemical code. The coupling of the two types of software is performed by developing a special code that has been written by using MATLAB. COMSOL Multiphysics is used to solve the coupled THMC processes (the C process is limited to solute transport) and PHREEQC is used to solve the geochemical reactions resultant of the transport of chemical species. Simulation results obtained by using the THM-GeoC simulator are compared with experimental data and data from modeling reactive transport, with good agreement in the results. The developed simulator is applied to investigate the coupled effect of climate changes and water enriched with carbon dioxide gas, which would be generated from low and intermediate nuclear wastes, on the dissolution of the limestone host rock in Ontario (Canada) for nuclear wastes, and porosity and permeability changes within the near field rock. The results show that the maximum change in porosity is approximately 3.5%, with a gradual decrease to approximately zero. The zone affected by the dissolution process is mainly located on the first 10 m within the host rock and does not cause a significant increase in permeability. From safety and environmental assessment perspectives, the impact of dissolution is not significant. However, parametric studies and experimental investigations need to be implemented to support the predicted results.

1. Introduction

Deep geological repositories (DGRs) that are used for the long term containment and isolation of nuclear wastes are considered as one of the most preferred technologies for the long term management of nuclear waste by preventing the transport of radionuclide into the biosphere. The main concept of the DGR system is that there are multiple natural geological and engineered barrier systems against radioactive transport into the biosphere for long life spans which are hundreds of thousands of years. Sedimentary rock formations as a natural geological host are currently proposed in several countries (e.g., Canada, France, and Switzerland). In Canada, a repository for low and intermediate levels radioactive wastes (LILWs) is being proposed by Ontario Power Generation (OPG) in limestone sedimentary rock formations in Ontario (Intera, 2011).

LILWs disposed in DGRs contain a wide range of chemical inventories (Quintessa and Geofirma, 2011). The long term degradation, reactions and mixing of LILWs with ground waters within repositories will lead to changes in the ground water chemistry and the generation of gases (e.g. carbon dioxide (CO_2), methane (CH_4), hydrogen (H_2), Geofirma and Quintessa, 2011; Fall and Nasir, 2011). The geochemical characteristics of ground water play an important role in the process of dissolution or precipitation within the pores of carbonate rocks, such as limestone (Engesgaard and Kipp, 1992; Rezaei et al., 2005). The process of precipitation and dissolution has an important role on the long term evolution of a DGR system with a natural barrier of limestone formation.

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Nomenclature

T	average temperature of the porous medium
Ceq	effective volumetric heat capacity
Keq	effective thermal conductivity
CL	volumetric heat capacity of the moving fluid
u	fluid velocity vector
ρ_f	fluid density
t	time
n	porosity
s	solid
f	fluid
κ	permeability
η	dynamic viscosity
p	pressure
D	direction of gravitational acceleration (g)
eff	volumetric deformation
K_D, K_S and K_f	bulk moduli of solid matrix, solid grains and water fluid, respectively
β, β_s and β_f	thermal expansion coefficients for the solid matrix, solid grains and water fluid, respectively
α'	$\frac{(\alpha-n)}{(1-n)}$
$\boldsymbol{\sigma}$	stress tensor
e_{ff}	volumetric deformation
C	concentration of total dissolved solids (TDS)
u_i, u_j	x and y direction displacements
D_L	hydrodynamic dispersion tensor
Sc	solute source or sink
G	shear modulus
λ	Lamé constant
γ_i	activity coefficient
z_i	ionic charge of the aqueous species
a_i^o	ion-size parameter
$SI_{Calcite}$	saturation index of calcite

Porosity and permeability are the key material parameters that control the (fluid, solute) transport processes in porous media. The evaluation of such changes is essential for any long term safety assessments related to DGR systems. The changes in permeability and porosity are directly affected by many processes, such as mineral phase dissolution/precipitation, or indirectly, such as the coupling impact of temperature to the rate of dissolution or precipitation. Predictions of the long term changes in porosity and permeability require the implementation of all relevant coupled processes, such as temperature, flow of water, fluid–waste or fluid–rock geochemical reactions, and mechanical stress and deformation. The investigation of such phenomena requires the development of a mathematical model and numerical tool that are able to capture and describe all relevant coupled thermo-hydro-mechanical-geochemical processes (Zheng and Samper, 2008; Taron et al., 2009; Zheng et al., 2010) that occur in the host rock of DGRs.

In general, numerous contributions have been made in the past years to develop single codes that deal with problems related to coupled processes in porous media or geo-systems. Furthermore, in recent years, there has been a steadily growing interest in coupling two or more codes (Jacques and Šimůnek, 2005; Taron et al., 2009; Wissmeier and Barry, 2011; Li and Fall, 2013a) to solve and model coupled processes in geo-systems because of the many advantages of this approach (coupled code) over the development of a single coupled computer code as described by (Jacques and Šimůnek, 2005; Taron et al., 2009; Wissmeier and Barry, 2011). Table 1 shows a list of common single and coupled codes that have been frequently used in the modeling of coupled processes or reactive transport in geo-systems. The mentioned works of research have significantly contributed to the understanding and the analysis of coupled processes or reactive transport modeling in geo-systems. However, most of the single or coupled computer codes described in Table 1 or developed during the past years cannot solve and describe all relevant coupled THMC processes that occur in the near field of DGRs for nuclear wastes. For example, many single (e.g., Zheng and Wang, 1998; Cheng and Yeh, 1998; Parkhurst and Appelo, 1999; Mayer, 2000; Xu et al., 2006) or coupled (e.g., Jacques and Šimůnek, 2005, Rutqvist and Tsang, 2003; Wissmeier and Barry, 2011) codes can only solve some of the coupled processes (e.g., HM, THC, THM) or THMC processes in an uncoupled or partially coupled way (e.g., HM, TH, THM, THC). Very few codes consider THMC coupled processes. For example, TOUGHREACT-FLAC3D (Taron et al., 2009) is one of the contributions that have investigated THMC coupled processes in porous media. TOUGHREACT-FLAC3D deals with the mechanical behaviour by a set of built-in geomechanical modules which are applicable to a wide range of geotechnical properties. On the other hand, the geochemical behaviour is solved by using a set of equations and data base files.

The objective of this paper is to develop a new coupled code that describes and assesses the THMC processes in the near field of DGRs and their impacts on the evolution of the rock porosity and permeability. In the current study, (COMSOL Multiphysics code Comsol, 2009) is used to solve the developed governing THMC partial differential equations (PDEs), and PHREEQC is used to solve geochemical reactions. In this developed approach, the geomechanical component of the code is fully coupled with the thermal, hydraulic and solute transport phenomena or processes. This results in the shortening of the execution times, thus improving computational efficiency (compared to linked codes where M is not fully coupled to TH), especially, when the geomechanics are not loosely coupled. The COMSOL–MATLAB interface facilitates users in accessing and interacting with the governing equations, non-linearity of material properties, solutions at different time steps and so many other options. The mentioned options make it possible to include more physics and processes in conceptual modeling. Moreover, this allows the easy implementation of future advances in constitutive relationships. In addition to that, the use of a well established geochemical code such as PHREEQC gives additional confidence to the developed model.

2. Simulator structure and coupling procedure

In this work, five coupled processes: thermal and mechanical processes, saturated flow, solute transport and chemical reactions are solved. The numerical modeling follows a two-step solution concept. First, a numerical model is developed to simulate the coupled THMC processes, in which the C represents the solute transport processes without chemical reactions. The second step is the geochemical reaction that takes place as a result of dynamic changes in the concentration resultant of solute transport as well as due to fluid–rock interaction reactions. The THMC model that is related to the first step is numerically solved by using COMSOL Multiphysics finite element (FE) code (Comsol, 2009) and the