Computers and Geotechnics 66 (2015) 219–229

Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Research Paper

Comparison of two simulators to investigate thermal–hydraulic–mechanical processes related to nuclear waste isolation in saliferous formations

Laura Blanco Martín [a,*], Ralf Wolters [b], Jonny Rutqvist [a], Karl-Heinz Lux [b], Jens T. Birkholzer [a]

[a] Earth Sciences Division, Lawrence Berkeley National Laboratory (LBNL), 1 Cyclotron Rd, MS 74R316C, Berkeley, CA 94720, USA
[b] Chair in Waste Disposal and Geomechanics, Clausthal University of Technology (TU Clausthal), Erzstr. 20, Clausthal-Zellerfeld 38678, Germany

ARTICLE INFO

Article history:
Received 23 September 2014
Received in revised form 23 December 2014
Accepted 30 January 2015
Available online 20 February 2015

Keywords:
Sequential modeling
Coupled processes
Benchmark
Heat-generating nuclear waste
Rock salt
Crushed salt

ABSTRACT

We investigate the capabilities of two simulators, TOUGH-FLAC and FLAC-TOUGH, to predict the long-term thermal–hydraulic–mechanical response of a generic salt repository for heat-generating nuclear waste. These simulators are based on sequential coupling and include state-of-the-art knowledge for saliferous materials. Their main difference is the sequential method used. We present a benchmark between LBNL and TU Clausthal. The scenario studied assumes heat and gas generation from the waste packages, and crushed salt backfill. The comparison of results is very satisfactory, providing increased reliability and confidence in the capabilities of the simulators to evaluate the geological and engineered barriers in the long-term.

1. Introduction

The underground disposal of nuclear waste requires the analysis of complex interactions between physical and chemical processes [1–6]. To comply with safety requirements, the performance of a nuclear waste repository has to be evaluated in the long-term (typically, thousands or even millions of years for heat-generating nuclear waste). Due to the complexity of the processes that need to be investigated, their interactions and the time scales considered, numerical modeling using proper tools and state-of-the-art knowledge is required [7].

Numerical modeling of coupled thermal–hydraulic–mechanical (and chemical) processes has been a frequent approach in recent years to tackle a wide variety of geosciences problems, including not only nuclear waste disposal, but also geological carbon sequestration, geothermal reservoir engineering and reservoir geomechanics [8–13]. Fully coupled and sequential approaches have been developed, implemented and improved as both computational capabilities and understanding of the involved processes have moved forward. Kim [14] and Olivella et al. [9] present extended descriptions of different formulations for coupled geomechanics and multiphase and heat flows. Fully coupled approaches are characterized by the simultaneous resolution of the governing equations of flow and geomechanics at each time step [9,15,16]. On the other hand, in sequential methods the flow and geomechanics sub-problems are solved one by one, using the intermediate solution information technique [17]. Different coupling strengths are possible when using sequential approaches, depending on how often the coupling between the two sub-problems is performed (i.e., at every iteration, at every time step or after a given number of time steps). The main advantages of sequential methods include the use of existing robust and well-established simulators for each sub-problem, the resolution of smaller systems of equations, the use of different time-stepping algorithms and the possibility to study different domains in each sub-problem [18–21]. When the sequential procedure is iterated at each time step until the solution converges, results from fully coupled and sequential schemes are the same [14]. However, while fully coupled approaches are unconditionally stable, stability and convergence are the key issues for the good performance of sequential schemes. In this respect, the fixed-stress split and the undrained split sequential methods are known to have favorable stability, consistency, accuracy and efficiency properties.

* Corresponding author. Tel.: +1 5104865456; fax: +1 5104865686.
E-mail addresses: lblancomartin@lbl.gov (L. Blanco Martín), ralf.wolters@tu-clausthal.de (R. Wolters), jrutqvist@lbl.gov (J. Rutqvist), karl-heinz.lux@tu-clausthal.de (K.-H. Lux), jtbirkholzer@lbl.gov (J.T. Birkholzer).

http://dx.doi.org/10.1016/j.compgeo.2015.01.021
0266-352X/Published by Elsevier Ltd.

In this research, we focus on sequential approaches to model coupled flow and geomechanics processes (i.e., thermal–hydraulic–mechanical, or THM) related to the underground disposal of heat-generating nuclear waste in saliferous formations. Although salt rock mass in principle does not have any connected pathways under undisturbed conditions and therefore is regarded as liquid and gas tight [2,6,22–24], the analysis of fluid dynamic processes in an abandoned repository (in particular, two-phase flow induced and affected by heat and gas generation from the exothermic nuclear waste packages, and also by the time-dependent convergence of the emplacement drifts) is of particular importance when investigating the long-term integrity (i.e., tightness or sufficient low permeability) of the geological and engineered barriers. Therefore, the development, verification and validation of suitable simulators are required for the analysis of THM coupled processes in a heat-generating nuclear waste repository in salt rock mass. In this research, we use two different sequential simulators, based on the same flow and geomechanics software, but relying on two different numerical schemes. The TOUGH-FLAC simulator has been developed at Lawrence Berkeley National Laboratory [11] and is based on a fixed-stress split method. The FLAC-TOUGH simulator, developed at Clausthal University of Technology [25], is based on an undrained split method. As their names suggest, both simulators use TOUGH2 for the non-isothermal, multicomponent and multiphase flow sub-problem [26], and FLAC^{3D} to solve the geomechanics sub-problem [27]. Since state-of-the-art constitutive relationships and coupling functions can be implemented with ease into these two simulators, they can be applied not only to model THM coupled processes in saliferous materials, but also to investigate a wide range of geosciences topics. One innovation of the updated simulators presented in this paper is that they use a Voronoi discretization in the flow sub-problem, even when the mesh deforms over time due to the creep and the large strains associated with the mechanical behavior of saliferous materials. We present results of a benchmark exercise between Lawrence Berkeley National Laboratory and Clausthal University of Technology. The principal objectives of this benchmark are to model the same scenario using the two mentioned simulators and to compare the results obtained. Indeed, it is acknowledged that, besides the validation of physical processes, the comparison of numerical results issued from different approaches and institutions increases confidence and reliability on the long-term predictions, and enhances acceptance of the conclusions reached [28]. In addition, such comparison leads to a code-to-code verification. Several benchmark projects to compare constitutive models for the thermal–mechanical behavior of rock salt have been reported in the literature [28–33]. Here, we focus on (1) the backfill evolution (in particular, reconsolidation process), on (2) processes that could affect the integrity of the host rock natural barrier at different temporal and spatial scales (i.e., temperature changes, damage, dilatancy and healing/sealing), and on (3) the effect of gas generation from the waste packages on the barriers integrity. We compare and analyze the capabilities of TOUGH-FLAC and FLAC-TOUGH to model the long-term coupled THM response of a repository for heat-generating nuclear waste in rock salt.

Rock salt is a potential medium for the underground disposal of nuclear waste because of several assets, including its water and gas tightness in the undisturbed state, its ability to creep and heal technically induced fractures and its relatively high thermal conductivity as compared to other shallow-crustal rock types [1,2,29,34,35]. In addition, rock salt is easy to mine, requires little reinforcement and can be found underground in large volumes in stable geological areas [28]. Furthermore, worldwide experience from the salt mining industry is available and includes construction know-how, long-term behavior of underground excavations in saliferous geosystems, geotectonic inventory of these geosystems and modes of failure mechanisms. With the aim of performing generic research that will support future site-specific work [36], we have considered a generic salt repository for heat-generating nuclear waste. Our repository assumes in-drift emplacement of the waste packages and subsequent backfill of the drifts with run-of-mine, granular salt. In this scenario, as the natural salt creeps under the effect of temperature and deviatoric stresses, the crushed salt backfill, which initially had a porosity of 30–45%, undergoes a reconsolidation process. It is expected that, when compacted, the crushed salt backfill will provide an additional (engineered) barrier role, thereby contributing to the natural barrier supplied by the host rock [37]. Indeed, during the reconsolidation process, the flow and mechanical properties of the crushed salt evolve towards the characteristic values of the natural salt [29,37,38]. As it will be discussed later, the evolution of some of these properties is currently well understood; however, the reconsolidation process at the high temperatures associated with heat-generating nuclear waste, as well as the effect of the moisture content on the compaction rate are currently under investigation [34,39]. Moreover, there are still some uncertainties about the remaining permeability and porosity of highly compacted crushed salt, as only a few experimental results are available [40].

This paper is organized as follows. First, we present the two sequential simulators used, TOUGH-FLAC and FLAC-TOUGH. Then, we present the new procedure to update the mesh in the flow simulation as the mechanical mesh deforms. The coupling between flow and geomechanics, including material-specific coupling functions for the crushed salt and the natural salt, is explained as well. The coupling functions that we use are based on current knowledge about the behavior of salt rock mass and granular salt under repository conditions for heat-generating nuclear waste, and will be improved as more data become available. Later, we give details on the benchmark exercise, and we compare and discuss the predictions obtained by the two simulators for the generic salt repository considered. The simulations include the stages of excavation, waste emplacement, backfilling and 100 000 years of post-closure. The comparison is very satisfactory, leads to a code-to-code verification, and demonstrates and provides confidence in the capabilities of the sequential approaches and simulators used to predict the long-term coupled THM response of a generic salt repository for heat-generating nuclear waste.

2. Materials and methods

The two simulators used in this research, TOUGH-FLAC and FLAC-TOUGH, present several similarities: (1) they are based on the same software (TOUGH2 and FLAC^{3D}), (2) they are both sequential simulators (i.e., the flow and geomechanics sub-problems are solved sequentially), (3) they can deal with large deformations, creep processes, non-isothermal, multiphase and multicomponent (at least, water and air) flow, and (4) they offer advanced constitutive relationships to model the time-dependent response of salt rock mass and granular salt. The main difference between these simulators is that they use two different methods to sequentially solve the flow and geomechanics sub-problems, as will be explained below.

2.1. TOUGH-FLAC for large strain and creep processes

The TOUGH-FLAC simulator [11] has been successfully used in many geosciences fields, and for the analysis of a wide range of geoengineering problems [10,11]. In order to investigate large strains and creep processes, TOUGH-FLAC has recently been updated [41]. One important update deals with the adaptation of the