Preliminary Simulation Analysis of the Large Scale Gas Injection Test (LASGIT) Experiment Using the OpenGeoSys (OGS) model

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Abstract: The OGS model is configured and used for simulation of the LASGIT project. The modeling conditions and the simulation results from the previous work by Walsh and Calder (2009) are analyzed to see if the simulation configuration is done correctly and to apply for the LASGIT project. Except for the unrealistic modeling conditions used previously, the simulation results successfully demonstrated helium propagation that is typical for the two-phase flow. The results indicated that the relations of capillary pressure and the relative permeability against water saturation used previously should be updated. An elaborated simulation with more realistic parameters should be used to improve the weak points of preliminary work.

Keywords: multi-phase flow, simulation, used nuclear fuel storage

Introduction

The LASGIT project is a full-scale test of gas transport in MX-80 bentonite clay at the Äspö Hard Rock Laboratory in Sweden (Sellin and Harrington, 2006). The experiment is based on the concept for deep geological repository for the spent nuclear fuel. The purpose of the LASGIT experiment is to improve the understanding of full-scale gas migration through the bentonite buffer under the repository conditions. For the purpose of the repository safety, an important question is whether the rate of gas generation and the consequent gas migration through the bentonite will decrease the effectiveness of the bentonite barrier. Laboratory research suggests that bentonite reseals upon resaturation (Cuss et al., 2011).

Walsh and Calder (2009) have focused on the gas injection portion of the experiment. They used a multi-phase flow and transport code, Transport Of Unsaturated Groundwater and Heat (TOUGH2) for simulation (Pruess, 1991). In their numerical simulation, they modified the code to simulate potential gas transport mechanisms. The modification is made mainly in micro- and macro- fracturing of bentonite by allowing pressure-induced changes to the bentonite

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permeability and capillary pressure.

Based on the previous work by Walsh and Calder (2009), numerical simulation is prepared for the LASGIT experiment in this paper. The simulation parameters is analyzed as a crucial step before any further simulation with the OGS model. The OGS model is a scientific open source project for the development of numerical methods for the simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media (Kolditz, et al., 2012a, 2012b). Among the OGS modules in the model, the experiment clearly involved the module of the two-phase flow through a bentonite barrier of the canister to an intact rock.

As in most cases of the two-phase flow, the fluid preference and competition toward the chosen media must be understood and represented through the relations between capillary pressure and saturation of the wetting phase fluid. Experimental work to study these relations is not commonly available in the literature. Therefore, the relations of capillary pressure and relative permeability are assumed as in the previous report (Walsh and Calder, 2009) and used for the preliminary simulation work in this paper. The objective of this work is to set up the OGS model for simulation of the LASGIT experiment and to analyze the first-off trial result to evaluate the applicability of the simulation configuration.

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Fig. 1. The spent nuclear fuel will be deposited at a depth of about 500 meters (Äspö hard rock lab).

Site Description

The spent nuclear fuel is to be deposited at a depth of about 500 meters as shown in Fig. 1. The barriers in the final repository consisted of canister, buffer (the bentonite barrier), and rock to prevent the radionuclides from being transported to the ground service. For monitoring of the half of the final repository, the pore pressure and total pressure responses are illustrated in Fig. 2.

Approach

The OGS model has basically two modules of the two-phase flow model depending on the choice of primary variables. The first is a typical choice of the wetting fluid pressure and the non-wetting fluid saturation, while the other is the capillary pressure of the wetting fluid and the non-wetting fluid pressure. The major difference of the two modules is found in Park et al. (2011).



Fig. 2. Qualitative illustration of the pore pressure and total pressure responses during the gas injection experiment (Walsh and Calder, 2009). LFA3 is an injection point.

Model Discretization and Property Assignment

A simple cylindrical problem domain is discretized with a preferential grid density applied in the bentonite material. The canister is not included in the problem domain, since no fluid flow occurs in it. The radial three dimensional grid is presented in Fig. 3. The bentonite is surrounded by the intact rock for a total model domain radius of 10 m. Vertically, the grid represents three meters of the bentonite from the bottom of the bentonite buffer to just above the middle injection port array in the canister. Due to the preferential grid density applied and the excluding of the canister itself, the resulting model domain has reduced a significant amount of computational units of the previous discretization. It consists of 9,842 nodes and 51,729 elements.

Boundary and Initial Conditions

The model has no-flow boundary conditions at the



Fig. 3. Discretized model domain (Only a half cut in the vertical direction).

top and bottom boundary of the model domain, and a fixed pressure boundary condition at the top perimeter. The actual pressure at the top perimeter outside the intact rock is not measured or known. Consequently, the fixed pressure boundary condition is determined assuming that the top of the model domain is open to atmosphere. This assumption is made from the handwritten schematics given for the analysis. However, only the perimeter of the top is used for the fixed pressure boundary to minimize the interference of a surface fixed boundary condition that may influence bentonite in the center and to let the model itself generate a hydrostatic condition vertically. Therefore, the fixed pressure boundary condition is determined by the depth (0 m), otherwise it is measured. Then, the two-phase flow model automatically generates hydrostatic conditions from the fixed boundary condition.

Initial conditions are important when the simulation model is sensitive to the initial guess in obtaining the next numerical solution of non-linear problems during iteration. In this simulation work, every primary variable is set to be zero initially, and the model establishes the initial hydrostatic condition right after the first iteration. However, more elaborated initial conditions are often required depending on extent of the nonlinearity in system.

Analysis on the Relations of Capillary Pressure and Relative Permeability against Water Saturation Used Previously

Since the previous simulation work was conducted

with TOUGH2 (Pruess, 1991), it is assumed that the parameters given by Walsh and Calder (2009) are summarized for the van Genuchten-Mualem model. The equations for the van Genuchten Mualem model are given as

$$P_{c} = -\frac{1}{\alpha} \left[S_{e}^{-1/m} - 1 \right]^{1/n} \tag{1}$$

$$k_{rw} = S_e^{\varepsilon} [1 - (1 - S_e^{1/m})^m]^2$$
⁽²⁾

$$k_{rnw} = (1 - S_e)^{\gamma} [1 - S_e^{1/m}]^{2m}$$
(3)

where n > 1, 0 < m < 1 and m = 1 - 1/n, α^{-1} is the inflection point (approximately P_e), $\varepsilon = 1/2$ and $\gamma = 1/3$ for pore connectivity. Then, the corresponding relations of capillary pressure and relative permeability against water saturation can be depicted in Figs. 4 and 5. Shown in the figures, the relations of water saturation and relative permeability for the bentonite and the intact rock are almost identical. This indicates that water does not likely move unless water saturation is above at least 50%, while helium likely moves starting from low values of gas saturation.

In addition, variations of capillary pressure for the both media are very little regardless of water saturation in Fig. 5. Most values are almost zero, which indicates almost no capillary pressure in the system. Then, water pressure and helium pressure are not significantly different. Whether the configuration is backed by experimental measurement is not known for this report. Note that the PcPnw module whose primary variables are capillary pressure and pressure



Fig. 4. van Genuchten Mualem relation of water saturation and relative permeability for bentonite and intact rock. Krl-B is the relative permeability of the liquid (water) for bentonite and Krg-B is the relative permeability of the gas (helium) for bentonite. Krl-I is the relative permeability of water for intact rock and Krg-I is the relative permeability of helium for intact rock.



Fig. 5. van Genuchten Mualem relation of water saturation and capillary pressure for bentonite and intact rock.



Fig. 6. Water pressure, helium pressure, and capillary pressure at 1,000 days.

of the non-wetting phase in the OGS model cannot be used when there exists no capillary pressure in the system. This means that there is no capillarity in the system, which does not represent the nature of twophase flow in a realistic way, unless two fluids are exactly same in Fig. 6.

Parameter	Unit	Bentonite	Intact rock
Permeability	m ²	1×10 ⁻²⁰	1×10 ⁻²¹
Porosity	-	0.4	0.002
Compressibility	Pa ⁻¹	3.2×10 ⁻¹⁰	3.4×10 ⁻¹⁰
van Genuchten n	-	1.82	1.88
van Genuchten P ₀	MPa	18	100

 Table 1. Medium properties

Table 2. Fluid properties

Fluid properties			
Property	Unit	Water	Helium
Density	kg/m ³	999.8	0.16674
Viscosity	Pa·s	9.772×10 ⁻⁴	1.956×10 ⁻⁵
Residual saturation	-	0.1	0.1
Maximum saturation	-	1.0	1.0

The medium properties are presented in Table 1. As for the fluid properties under isothermal conditions, water and helium at atmospheric conditions are assumed in Table 2. Note that there is more than three orders of magnitude difference in density between water and helium.

Gas Injection Test Modeling

As shown in Fig. 6, there is almost no pressure difference between the wetting fluid and the nonwetting fluid due to the absence of capillary pressure given the previous relations of capillary pressure and the wetting phase saturation. This causes a serious problem to assess helium saturation at the injection port. For instance, the injection pressure (2.5 MPa) of helium or water at LFA3 cannot be calculated back to the corresponding capillary pressure and further water or helium saturation, unless the injected helium saturation at LFA3 is assumed. Therefore, an arbitrary injection saturation (25%) of helium is assumed with the same injection pressure at LFA3.

The total simulation period is 1,010 days. Pressure of water and helium over the simulation period is provided in Fig. 7 for the ports of UR903, 904, 905, and 906. In general, pressure increases gradually over the simulation period.

Similar to Fig. 7, pressure over the simulation time at the ports of UR907, 908, 909, and 910 increases gradually, while those ports nearer to LFA3 (the injection point) are higher pressure zones in Fig. 8.

As expected, pressure at LFA3 itself is steady at 2.5 MPa over the simulation period in Fig. 9.

the corresponding helium Finally, saturation (propagation) for the given initial and boundary conditions at 1,010 days is depicted in Fig. 10. Since the maximum helium saturation value at the injection port (LFA3) is set as 0.25, the value has never gone higher than 0.25. Nevertheless, the propagation volume of influence is about the same given the simulation conditions. The helium propagation volume is still within the bentonite barrier as in the work by Walsh and Calder (2009). This indicates that ambient pressure difference generated by the injection is more or less within a reasonable magnitude of difference from the previous simulation condition in the work by Walsh and Calder (2009).



Fig. 7. Water and helium pressure at 1,000 days.



Fig. 8. Water and helium pressure at 1,010 days.



Fig. 9. Water and helium pressure at 1,010 days.



Fig. 10. Injected helium saturation at 1,010 days.

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Summary

The preliminary work for simulating the LASGIT experiment using the OGS model is conducted in this paper. In spite of the difficulty in accessing full simulation data and conditions with respect to the previous work by Walsh and Calder (2009), the model configuration is successfully achieved for further elaborated simulations in need.

Obviously, the present study should be adjusted to better analyze against the previous work. Particularly, the relations of capillary pressure and relative permeability against water saturation used previously should be updated. This adjustment should enable the PcPnw module to work properly as well. Once the adjustment is successfully made, further coupling with mechanical deformation for a material failure analysis would produce more meaningful and precise results.

Acknowledgments

I acknowledge the funding by Basic Research Program at Korea Institute of Geoscience and Mineral Resources and comments by Dr. Robert Walsh. I also thank the anonymous reviewers for their fruitful reviews.

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Manuscript received: July 5, 2012

Revised manuscript received: August 2, 2012

Manuscript accepted: August 23, 2012