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The Petroleum Engineering Department Presents

Analytical Modeling of Bentonite Swelling and Numerical Reactive Transport Modeling in Nuclear Waste Disposal Systems

Xinwei Xiong

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Location: UH Technology Bridge, Building 9A, Room 124

Committee Chair:

Kyung Jae Lee, Ph.D.

Committee Members:

Mohamed Soliman, Ph.D. | Michael T. Myers, Ph.D. | Lori Hathon, Ph.D. | George K. Wong, Ph.D.

Abstract

Bentonite has been widely used as buffer and backfill materials for nuclear waste disposal in last few decades. The main reasons of bentonite being selected for buffer and backfill materials include its low hydraulic permeability and high plasticity, which can restrict the transport of nuclear waste through the barrier and maintain the sealing ability of barrier even with the deformation of bentonite, respectively. Montmorillonite is considered as the primary constituent of bentonite, which is a major expandable mineral. However, many researches have proved that hydrated cations in the montmorillonite are able to be exchanged by K+ in pore fluid at high temperature and form illite. This illitization process would reduce the

amount of montmorillonite in the bentonite. Since illite is an unexpansive clay mineral, illitization may result in cracking on the barrier and subsequently increase the risk of nuclear leakage.

In this dissertation, to investigate how illitization process affect swelling capacity of bentonite buffer and safety of nuclear waste disposal system, I have completed the following three tasks: (1) Propose an optimized analytical solution to describe the water movement and clay swelling by taking account of porous media deformation, through experimental validation with different mass fractions of montmorillonite. From the hydrothermal reaction experiment, the relationship between illitization reaction rate and concentration of K^+ is analyzed. (2) Determine the reactive transport properties of bentonite in nuclear disposal systems through the pore-scale modeling of smectite illitization and clay deformation, by examining the changing pore volume, reaction rate, and effective diffusion coefficient as a function of porosity and temperature. (3) Develop a macroscale model by using the reactive transport properties obtained from the pore-scale modeling, and validate the results with research-purpose software, TOUGHREACT. Through this, feasibility to replace the complex simulation of TOUGHREACT with the developed simplified macroscale model will be determined. In addition, the long-term behavior of nuclear waste disposal system is predictably analyzed.

As such, this dissertation research includes the whole workflow of conceptually analyzing the bentonite clay swelling process with analytical modeling, quantifying the changing mineral compositions of bentonite by hydrothermal reaction experiments, and numerically modeling the reactive transport process of smectite illitization in bentonite buffer of engineering barrier system from pore-scale to macroscale. The findings are expected to provide reliable solution for safe nuclear waste disposal with engineering barrier systems.