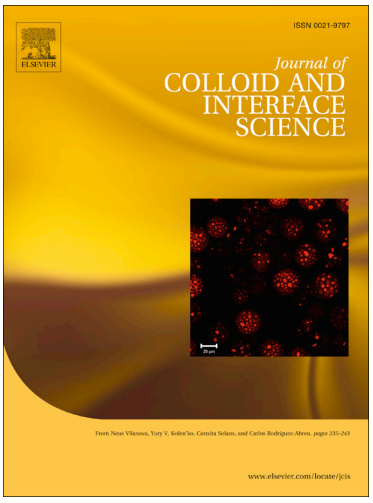

Pore-scale study of thermal effects on ion diffusion in clay with inhomogeneous surface charge

Yuankai Yang, Moran Wang

PII: S0021-9797(17)31437-6
DOI: https://doi.org/10.1016/j.jcis.2017.12.047
Reference: YJCIS 23119

To appear in: *Journal of Colloid and Interface Science*

Received Date: 29 September 2017
Revised Date: 25 November 2017
Accepted Date: 17 December 2017

Please cite this article as: Y. Yang, M. Wang, Pore-scale study of thermal effects on ion diffusion in clay with inhomogeneous surface charge, *Journal of Colloid and Interface Science* (2017), doi: https://doi.org/10.1016/j.jcis.2017.12.047

Pore-scale study of thermal effects on ion diffusion in clay with inhomogeneous surface charge

Yuankai Yang and Moran Wang[1]

Department of Engineering Mechanics and CNMM, Tsinghua University, Beijing 100084, China

Abstract

A better understanding of thermal effect on ion transport in compacted clay is of great significance to enhance long-term safety of repository for high-level radioactive waste. It was reported that the macroscopic Soret coefficient in clay is five times larger than that in free water, which was ascribed to the electrokinetic effect. By pore-scale simulations using lattice Boltzmann method, it is found that the Soret effect contributes little to the ionic flux changes in clay because the Soret coefficient is still around the value in free water for different external temperature gradients. The essential cause is the inhomogeneous charged liquid-solid interfaces in clays induced by the temperature gradient. This interface effect plays an important role to the significant changes of inner electrical and concentration fields in clay. Therefore the concentration diffusion and electromigration should be responsible for this phenomenon instead of the thermodiffusion (Soret effect). This study may improve understanding of ion transport in clays driven by multiphysiochemical effects.

***Keywords*:** Soret coefficient; thermal effect; electrokinetic transport; inhomogeneous charged surface; compacted clay

[1] Corresponding author. Tel: 86-10-627-87498; E-mail: mrwang@tsinghua.edu.cn (M. Wang)