Impact of microstructure on anion exclusion in compacted clay media
Christophe Tournassat, Stéphane Gaboreau, Jean-Charles Robinet, Ian C. Bourg, Carl I. Steefel

To cite this version:
Christophe Tournassat, Stéphane Gaboreau, Jean-Charles Robinet, Ian C. Bourg, Carl I. Steefel. Impact of microstructure on anion exclusion in compacted clay media. Euroclay 2015, Jul 2015, Edinburgh, United Kingdom. <hal-01137606>

HAL Id: hal-01137606
https://hal-brgm.archives-ouvertes.fr/hal-01137606
Submitted on 31 Mar 2015
Impact of microstructure on anion exclusion in compacted clay media

Christophe Tournassat¹²*, Stéphane Gaboreau¹, Jean-Charles Robinet³, Ian C. Bourg⁴, Carl I. Steefel²

¹Water, Environment and Ecotechnology Division, French Geological Survey (BRGM), Orléans, 45060, France
²Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States
³Research and Development Division, Andra, Châtenay-Malabry, 92298, France
⁴Department of Civil and Environmental Engineering, Princeton University, Princeton, NJ 08544, United States

*Corresponding author: Christophe Tournassat, BRGM, D3E/SVP, 3 avenue Claude Guillemin, 45060 Orléans Cedex 2, France. E-mail: c.tournassat@brgm.

Abstract

The sensitivity of ion concentration distribution models to three key model assumptions, the pore-size distribution of clay media, the distance of closest approach of ions to the clay surface, and the accessibility of sub-nanometer-wide clay mineral interlayer spaces to anions, was explored by solving the Poisson-Boltzmann equation for swelling and non-swelling clay materials. Our calculations show that all three model assumptions significantly impact values predicted for the anion accessible porosity. As a consequence, macroscopic measurements of anion exclusion in clay media cannot be used to test any of the three model assumptions independently of the two others. Information gained at the nanoscale, in particular, a detailed characterization of pore size distribution, is necessary to develop accurate predictive models of the anion accessible porosity of clay media.

Keywords: clay, illite, montmorillonite, anion exclusion, Poisson-Boltzmann, microstructure, molecular dynamics.