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A three-scale computational model of reactive pollutant transport in smectitic clays

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SUMMARY

A three-scale model of dual-porosity type is proposed to describe contaminant transport in swelling clays. The swelling medium is characterized by three separate length scales (nano, micro and macro) and two levels of porosity (micro- and macro-pores). At the nanoscale the medium is composed of charged clay particles saturated by a binary monovalent aqueous electrolyte solution occupying the micro-pores. At the intermediate (micro) scale the two-phase system is represented in a homogenized fashion with averaged microscopic equations governing the behaviour of the clay clusters (or aggregates) regarded a two-phase mixture composed of clay particles and electrolyte solution. At the macroscale, the microscale mixture of clay clusters is homogenized with the bulk solution containing non-electrolyte species lying in the macro-pore system. The resultant macroscopic picture appears governed by a dual-porosity model wherein the clay clusters act as sources/sinks of mass to the macro-pore system. Under a local equilibrium assumption between the clay clusters and macro-pores, a quasi-steady version of the dual-porosity model is derived. This framework combined with a three-scale picture of the colloidal system allows to provide nanoscopic representations for the retardation coefficient, governing the instantaneous adsorption/desorption of the ionic species in the micro-pores, in terms of the local behaviour of the electrical double layer potential which satisfies a Poisson–Boltzmann-type problem at the nanoscale.

KEY WORDS: active clays; homogenization; dual porosity; adsorption; retardation coefficient; electrical double layer; Poisson–Boltzmann

1. INTRODUCTION

Swelling porous media such as 2–1 lattice clays, hydrophilic polymers, shales, and connective biological tissues are ubiquitous in almost all aspects of life. For example, clay is one of the

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