Geophysical Research Abstracts, Vol. 7, 10156, 2005
SRef-ID: 1607-7962/gra/EGU05-A-10156

Dual continuum models of fully coupled non-isothermal multiphase flow and reactive transport in porous media

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Double porosity, double permeability and dual continuum models (DCM) are widely used for modeling preferential water flow and mass transport in unsaturated and fractured media. Here we present a DCM of fully coupled non-isothermal multiphase flow and reactive transport model for the FEBEX compacted bentonite, a material which exhibits a double porosity behavior.. FEBEX (Full-scale Engineered Barrier EXperiment) is a demonstration and research project dealing with the bentonite engineered barrier designed for sealing and containment of a high level radioactive waste repository. Our DCM considers inter-aggregate macro-pores, and intra-aggregate and interlayer micro-pores. Two types of DCMs are tested: the dual continuum connected matrix (DCCM) and the dual continuum dis connected matrix (DCDM). Liquid flow in macro-pores is described with a mass conservation equation accounting for Darcian flow, chemical and thermal osmosis. In DCCM, water flux in micropores is calculated with a modified Darcy's law by adding a chemical osmosis term. A simple mass balance equation is used for DCDM which contains a storage and a water exchange term for water in micropores. A mixed type of water exchange term is adopted which includes a second order term accounting for water transfer due to the difference in liquid pressure and a first order term accounting for the gradient in chemical osmosis pressure. Equations of mass conservation for liquid, gas and heat in macropores and liquid mass conservation in micropores are solved by using a Newton-Raphson method. Two transport equations with a coupling interaction term are used to describe solute transport in macro- and micro-pores. The coupling term contains a first order diffusion term and a convection term (solute exchange due to water exchange). Transport equations as well as chemical reactions in the two domains are solved by means of a sequential iteration method. All these feature have been implemented in a finite element code

(INVERSE-FADES-CORE). The formulation has been applied to the interpretation of a long-term permeation test performed on a sample of FEBEX bentonite.