ABSTRACT

Title:	MIN3P-THCm Code Enhancements for Reactive Transport
	Modelling in Low Permeability Media
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Abstract

The reactive transport code MIN3P-THCm was enhanced by strengthening its simulation capabilities for geochemical processes in low permeability porous media in which transport is diffusion-controlled. Code enhancements include a multisite ion exchange (MIE) model, a multicomponent diffusion (MCD) model, and a hybrid multicomponent diffusion (hMCD) model. Simulation capabilities were further extended by implementing domain discretization in radial coordinates, in addition to standard Cartesian coordinates. The code enhancements are useful for simulating reactive transport in engineered barrier systems and in low permeability host rock considered for deep geological repositories. This report documents the theoretical background, the governing equations, and the numerical implementation for these new ion exchange and diffusion modules. In addition, relevant sections of the updated user guide are described and verification examples for evaluation of the simulation capabilities are provided.