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Original article

Fully coupled algorithm for heat and water transport – Estimation of non-linear parameters based on the experimental data

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Abstract

We solve the problem of coupled heat conduction and water transport in bentonite with water present in vapour and adsorbed form in a non-equilibrium state. The problem is governed by a system of two parabolic PDE and one ODE. Most of the coefficients are non-linear functions, defined either by underlying physical phenomena or empirically. We present a numerical scheme using FEM with linear base functions, implicit time discretization, and simple iterations for the non-linear terms. The model is verified against experiments (one 1D and one 3D) and we demonstrate the use of optimization algorithm for parameter calibration. Some of the parameters could be estimated successfully while others with limited confidence, which is explained by the particular character of the non-linear parameter dependence and resulting small sensitivity of the model on some parameters.

Keywords: Coupled processes; Monolithic scheme; Parameter calibration; Water adsorption

1. Introduction

The motivation of this work comes from deep geological disposal of spent nuclear fuel. The repository concept considers compacted bentonite buffer as engineered barrier, employing the bentonite swelling and sorption ability. Besides other processes, the thermo-hydro-mechanical (THM) processes are studied, which are strongly coupled in the given conditions and make a challenge for modelling from both of views of numerical methods and model data acquisition.

One of the challenges in the THM simulation of clay materials is representation of water forms. In contrast with other porous media, water in clay materials is in significant part present in the adsorbed (chemically bound) form in the solid grains (matrix), besides the liquid and vapour in the pore volume considered in the standard models of multiphase porous media flow. The models used for study of THM behaviour of bentonite as the repository buffer material typically use empirical equivalent of unsaturated porous media, where all the present water is considered as liquid with the description by means of retention curve (relation between saturation and negative (suction) pressure) [8]. An attempt to consider more physically based model of water transport in bentonite has been done by Krohn [4] – the vapour diffusion and non-linear equilibrium adsorption in the solid phase. The simulation code developed by the above cited author himself is limited to 1D case. The preceding work of authors [3] present the model similar to that

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