A THMC FRAMEWORK TO CONSIDER MICROSTRUCTURAL EFFECTS IN THE ANALYSIS OF CLAY BARRIERS

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ABSTRACT

Clay barriers envisaged for the isolation of nuclear waste have several aims: to provide mechanical stability to the canister, to delay water arrival and to retard and/or retain the radionuclides released when the canister deteriorates. Integrity and good performance of the barrier depend on thermal, hydraulic, mechanical and chemical conditions. In consequence, the numerical modelling of coupled THMC (thermo-hydro-mechanical and chemical) phenomena is an important tool for design, interpretation and prediction for the short and long term behaviour of this type of isolation system. A common feature of the formulations commonly used in coupled analyses is the assumption of the clay barrier as a single porosity material. However, the pore structure of expansive clays presents more than one type of voids. In the last few years, a number of tests have been performed revealing a strong influence of the pore structure on the behaviour of expansive clays (e.g. Lloret et al. 2003). Therefore, a proper modelling of a clay-based engineered barrier should incorporate a fully coupled THMC formulation within a double structure framework that takes into account the individual THMC behaviour of micro and macro structures of the swelling clay and the possible interactions between them. In this kind of formulations there are two types of couplings: between the physics problem (THMC behaviour) and between the structural levels of the material (micro and macro structures).

In this contribution, a formal mathematical framework is used to model the Thermo-Hydraulic-Mechanical and Chemical (THMC) behaviour of compacted bentonite in laboratory scale tests. First, a simple single porosity model is used to simulate the test. The THMC (single porosity) formulation (Guimaraes et al. 2005) generalizes an existing THM code (Olivella et al., 1995) by incorporating the reactive transport equations in an unsaturated deformable porous medium. The formulation is fully coupled allowing, therefore, the examination of the interactions between the various phenomena present in the barrier. The chemical equilibrium equations are solved by ensuring the minimization of Gibbs free energy. This approach allows the use of robust optimization algorithms that contribute significantly to the overall efficiency of the analysis. Special attention is given to heterogeneous reactions involving solid and liquid phases such as cation exchange and precipitation/dissolution of minerals. The results are critically analysed discussing the capabilities and limitations of this model.

The numerical modelling of the (THMC) behaviour of unsaturated expansive clays requires not only coupled flow relationships accommodating a number of mechanisms (heat transfer, moisture transfer, gas flow, swelling, chemical transfer, etc); but also the adoption of a conceptual model closer to the actual material characteristic. Therefore, the paper also proposes the extension of the original (single porosity) model to a double structure framework that would allow the adoption of a more realistic conceptual model for the description of the clay behaviour and the clay-water system. The double structure model (Sánchez et al., 2005) considers the existence of two pores structures (the macrostructure and the microstructure) and is able to reproduce the main characteristics of expansive clays behaviour, such as the dynamic character of the expansive clay fabric observed during hydration. The explicit inclusion in the constitutive law of these two basic structural levels, and their main interactions, provides a powerful approach to analyse and to describe the behaviour of expansive clays. The constitutive law has been formulated in the context of elasto-plasticity for strain hardening materials. A well-known elasto-plastic model for unsaturated soils,
which describes the macrostructural behaviour, has been combined with a generalized plasticity model to reproduce the irreversible effects characteristic of expansive clays.

Finally, the double structure model has been extended to incorporate chemical effects. An interesting feature of the model is the assumptions that chemical changes affect only the microstructural behaviour. These changes, however, have macrostructural effects through the interaction between the two structural levels. To advance in the knowledge of the behaviour of this bentonite, tests in thermo-hydraulic cells were carried out by CIEMAT. The thermo-hydraulic cell analysed herein (coded as CT-17, Villar et. al., 1997) try to reproduce the thermal, hydraulic, mechanical and chemical conditions prevailing in a clay barrier made up of compacted bentonite blocks. The clay was uniaxially compacted inside a stainless steel cell (Figure 1) with an initial dry density of 1.65 g/cm³ and an initial water content of 13.7 %. The resulting compacted bentonite block has a diameter of 15 cm and a height of 14.6 cm. The bottom of the cell has two hydration ports leading to a porous plate, through which deionized water at a pressure of 1 MPa is injected by an automatic pump. In the upper part, an axial heater 10 cm length is placed. The temperature at the heater surface was fixed at 100 °C. Post-mortem analysis of the cell gave relevant information of the behaviour of the bentonite after the test and this information was used to validate the numerical model (Figure 2).

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References


