COUPLED THMC MODEL OF FEBEX MOCK-UP TEST

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INTRODUCTION

FEBEX (Full-scale Engineered Barrier EXperiment) is a demonstration and research project dealing with the bentonite engineered barrier designed for sealing and containment of waste in a high-level radioactive waste repository (ENRESA, 2000). It includes two main experiments: an in situ full-scale test performed at Grimsel (GTS) and a mock-up test operating since February 1997 at CIEMAT facilities in Madrid (Spain). One of the objectives of FEBEX is the development and testing of conceptual and numerical models for thermal, hydrodynamic, mechanical, and chemical (THMC) processes taking place in engineered clay barriers. The mock-up test provides valuable insight on simultaneous heating and hydration at large scale because it is performed in conditions much better controlled than those of in situ test. Hydration of bentonite barrier involves complex interactions among thermal, hydrodynamic, mechanical and chemical processes. A coupled THMC model of the mock-up test is presented here.

MODEL SETUP

Multiphase flow processes considered in the model include: 1) coupled flow of liquid water under hydraulic, chemical and thermal osmosis gradients, 2) flow of vapor (advection and dispersion), 3) flow of gaseous species other than steam (advection and dispersion), 4) flow of air dissolved in water (advection), and 5) transport of heat through liquid and gaseous phases (convection) and solid skeleton (conduction). Bentonite swelling is solved by a state-surface approach. Chemical processes include: aqueous complexation, acid-base, mineral dissolution/precipitation, gas dissolution/exsolution, cation exchange and surface complexation. The spatial domain is discretized with 1-D axysymmetric mesh of rectangle finite elements (Figure 1). Intrinsic and thermal osmotic permeabilities are estimated by solving the inverse problem using INVERSE-FADES-CORE (Zheng and Samper, 2004).

MODEL RESULTS

Simulations have been performed for several conceptual models (scenarios) which are listed in Table 1. Good agreement between measured and computed relative humidities at several radial distances as well as cumulative water inflow are observed over the whole time scale, although computed humidities near the heater underpredict measured values. The best fit to measured cumulative water inflow is achieved with a THMC model with variable permeability (Kozeny’s Law) and thermal osmosis (see Figure 2).

![Figure 1: Finite element mesh and boundary conditions used in the numerical model. T is temperature, P is liquid pressure, u is displacement in radial direction and v is the displacement perpendicular to radial direction.](image-url)
Figure 2: Measured (symbols) and computed cumulative water inflow for scenarios listed in Table 1.

<table>
<thead>
<tr>
<th>Scenario 1 (ENRESA, 2000)</th>
<th>Scenario 2 (Samper et al., 2005b)</th>
<th>Scenario 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intrinsic permeability</td>
<td>2.75·10^{-21} m²</td>
<td>K = 3.51·10^{-21} \left(\frac{\phi}{(1-\phi)^2}\right)^2 \frac{(1-0.41)^2}{0.41^3} m²</td>
</tr>
<tr>
<td>Thermal osmotic permeability</td>
<td>7.5·10^{-13} m²/K·s</td>
<td>3.62·10^{-12} m²/K·s</td>
</tr>
<tr>
<td>Mechanical deformation</td>
<td>No</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Long term predictions (200 years) indicate that hydration of bentonite barrier will be a very slow process as long as heating is maintained. Predicted spatial distribution of main chemical species, minerals and exchangeable cations are presented. Dilution induced by hydration and concentration increasing induced by evaporation are the two main processes controlling the spatial distribution of conservative species. Chloride concentrations do not reach steady state even after 30 years of heating and hydration due to the extremely low hydration rate (Zheng, 2006).

ACKNOWLEDGMENTS
This work has been funded by ENRESA and European Union under contracts PI4W-CT95-0006 and FIKW-CT-2000-0016. Partial funding was provided also by Spanish Ministry of Science and Technology (CICYT, HID98-282) and University of La Coruña through a research scholarship awarded to the first author.

References: