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Inspecting the role of vapour loss and other model strategies in the modelling of a bentonite thermo-hydraulic cell

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Models of engineered bentonite barriers in radioactive waste repositories need to use conceptual and numerical models that consider the most relevant processes taking place. To study such processes, numerous laboratory experiments have been carried out. In this work, we will model the thermo-hydraulic cell presented by Pintado and Lloret [6], since it allows the study of a simple thermo-hydraulic heating test with limited influence of other phenomena. The aim of the study is to conduct several modelling exercises to inspect in a simple way the relevance of different model aspects in this case, such as dimensions simplification and porosity levels, and processes, such as hydraulic and mechanical coupling, water vaporisation and, especially, vapour loss.

In the modelled test [6], a cylindrical Febex bentonite specimen (diameter 38 mm, height 78 mm) was subject to heating for 7 days. Initially, the sample had a dry density of 1.63 Mg/m^3 and a water content of 15.3%. A constant heater power of 2.17 W was applied on one end of the sample. At the other end, the temperature was kept constant at 30 ºC. The sample was surrounded with an insulation cover, and the external temperature was of 25 ºC. Temperature was recorded in points of the specimen located at heights z = 0, 20, 38, 60 and 78 mm (Figure 1).

The first modelling exercise conducted is a 1D study solving the steady-state thermal problem in a finite rod, using an analytical solution [1]. Only the bentonite was modelled, and the insulation is introduced as a lateral loss boundary condition. Then, the only parameters needed are the dimensions of the sample (length, section area A, perimeter), the external temperature, the thermal conductivity of bentonite and thermal conductance of the insulation. The conductivity of bentonite is taken as homogeneous and constant equal to 1.13 W/m/K. This exercise identified the conductance of the insulation as 1.09 W/m^2/K, which is of the same order of magnitude as that identified by Pintado et al. [5]. In addition, since part of the generated heat is not transferred to the bentonite sample, an efficiency factor to the heater power has been identified of 0.39 to fit the steady-state temperatures. This is consistent with the estimated 60% power loss pointed out by Pintado and Lloret [6].

Subsequently, the transient 1D thermal problem was modelled. The heat equation was numerically integrated in Matlab. A constant global heat capacity of the sample c_G was computed for the initial conditions as the weighted component average [4], taking into account the solid phase, liquid water and vapour. The specific heat capacity values used are c_S = 1091 J/kg/K, c_L = 4184 J/kg/K and c_V = 1900 J/kg/K, for the solid, liquid and vapour components, respectively. The result is c_G = 1100 J/kg/K. This model does not accurately capture the transient experimental temperature values (Figure 1).

Further complexity was then introduced in the model to discard some effects as responsible for the poor fitting to the transient problem. A 2D axisymmetric finite element model was built, solving the thermo-hydro-mechanical problem, with double porosity retention curve as in Navarro et al. [3]. The hydraulic problem included water vaporisation, and the transport of liquid and vapour. The thermal problem was solved as the balance of enthalpy per unit volume h as a sum of component enthalpies [2], taking into account the solid phase, macrostructural liquid water, microstructural water and vapour. A Neumann boundary condition was used for the heater power with the identified efficiency factor, and the heat loss through the insulation was introduced as a Neumann boundary condition with the identified conductance. The thermal conductivity of bentonite was computed as the weighted average

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between saturated (1.28 W/m/K) and dry thermal conductivities (0.57 W/m/K) [7]. The obtained temperatures were not very sensitive to these changes, since they are similar to the transient 1D thermal problem (Figure 1). The experimental transient results were still not accurately reproduced. This can lead to think that additional heat losses occur that are not considered, such as vapour leakage. Pintado and Lloret [6] estimated a vapour leakage of 0.1 g/day in the test.

Finally, the vapour mass needed to be lost for the model results to reproduce the transient recorded temperatures was estimated. To this end, the evolution of gained enthalpy H in the bentonite sample was studied in the numerical model and from the temperatures recorded, and both were compared. In the numerical model, H_{model} was obtained by integrating h in the sample volume for all the solved times. For the experimental results, experimental temperature T_{exp} profiles were integrated for several times to obtain H_{exp} as $\int_0^{0.078} A\, c_G \left(T_{\text{exp}} - T_0\right) \mathrm{d}z$, where T_0 is the initial value of temperature. The difference between H_{model} and H_{exp} is the greatest around 2 h. The mass of leaked water vapour m_v that would cause such an enthalpy sink can be computed as $(H_{\text{model}} - H_{\text{exp}})/h_v$, where h_v is the specific enthalpy of vapour. For the time 2 h, the obtained m_v is 1 g, which gives a constant leakage rate to that time of 15 g/day. Comparing this value to the 0.1 g/day reference [6], it is higher by 2 orders of magnitude, which makes it unlikely that the cause for the discordance between model and experimental temperature results is vapour leakage alone.

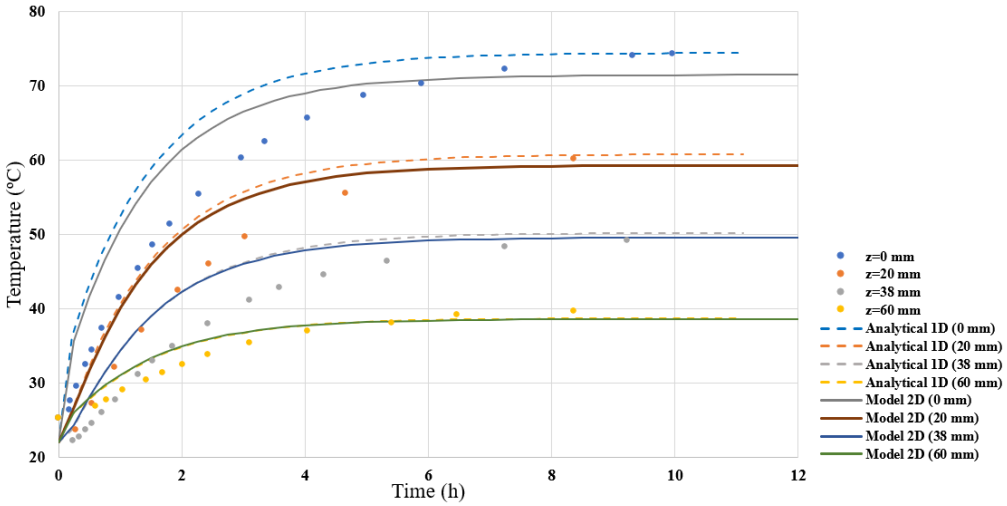

Figure 1: Evolution of temperature with time in the 5 sensor positions. Markers: experimental values. Dashed line: 1D transient model. Solid line: 2D axisymmetric model.

Contributor statement

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