A Large Deformation Model with Strong Chemical-Mechanical Coupling for Bentonite to Assess the Bentonite Buffer Behaviour in Spent Nuclear Fuel Disposal Conditions

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Introduction

Modelling the deformation of bentonite in a state where it has structure requires a continuum mechanical model. To include the contribution of water movement and salinity to this model requires the use of continuum thermodynamics leading to a so-called continuum thermomechanical model. The model has to be formulated in a large deformation mathematical setting, since bentonite can swell highly (the strain is higher than a few per cent in the most of the applications). In this work, the conceptual and mathematical basis for this type of model for bentonite is formulated and a few example simulations are presented to illustrate the capabilities of the model. The swelling by lowering salinity covered by the model corresponds to the starting of erosion in dilute water conditions.

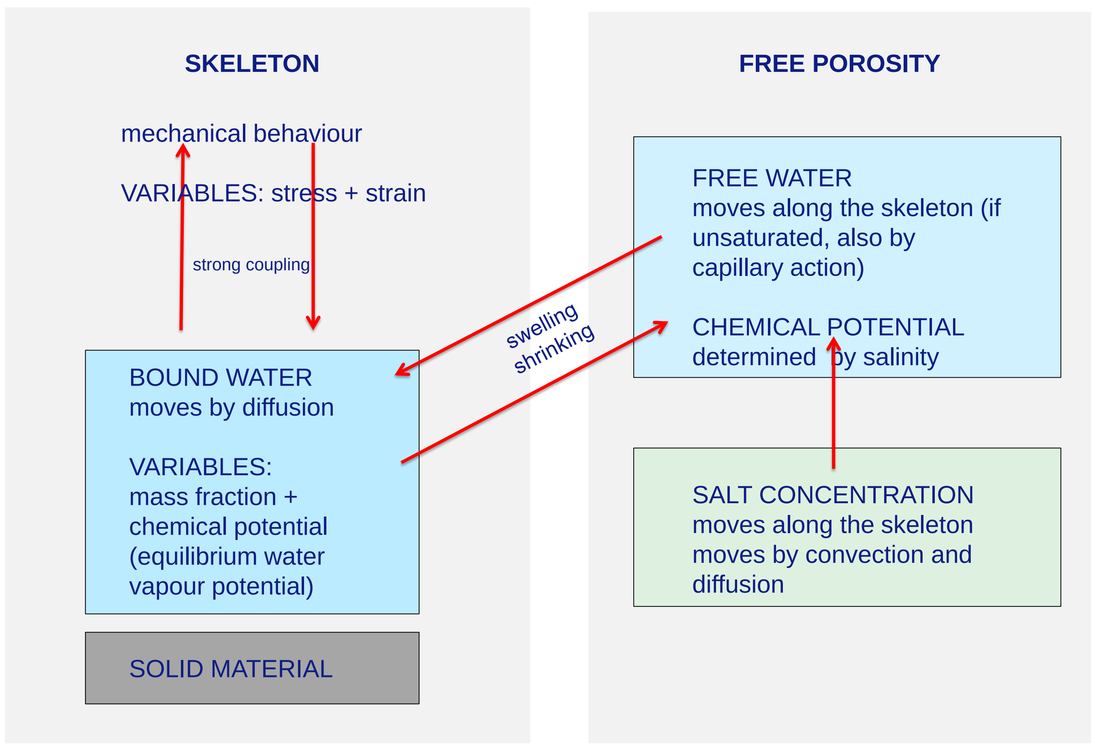

Figure 1. An illustration of the model concept and couplings.

Concept

The model concept and couplings are illustrated in Figure 1.

The work-conjugate variable pairs used in the model for the bentonite skeleton are

- stress (2nd Piola stress) – strain (right Cauchy-Green deformation tensor) for the mechanical deformation
- water mass fraction – chemical potential for the bound water

between which a two directional strong coupling is formulated using the basic principles of thermomechanics.

In the free porosity

- free water moves along the skeleton (or by capillary action in unsaturated state)
- salt (NaCl) moves along the skeleton and by convection-diffusion

The exchange of water between the bound state and the free pore water causes the swelling. The exchange is determined by the potential energy difference of the waters. The stress-strain state contributing to the bound water potential, the swelling stops when the mechanical energy is in balance with the chemical potential difference of the waters.

An example simulation

The simulation demonstrates swelling of a fully saturated bentonite sample 1) when the outer boundary of confined bentonite body is freed and the bentonite let to swell into artificial fracture and 2) during two steps of salinity decrease on the outer edge. The parameters of this simulation are not for any particular bentonite type and the scales are not necessarily accurate.

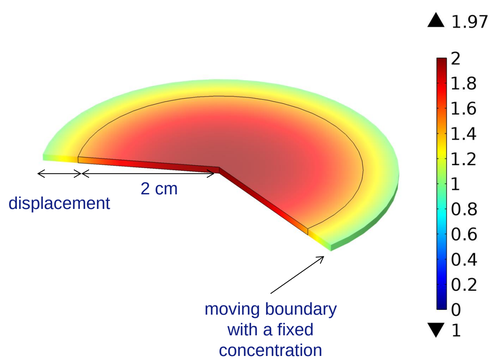

Figure 2. Model geometry and example of the concentration profile (mol/l) at t=190 d (time is not scaled).

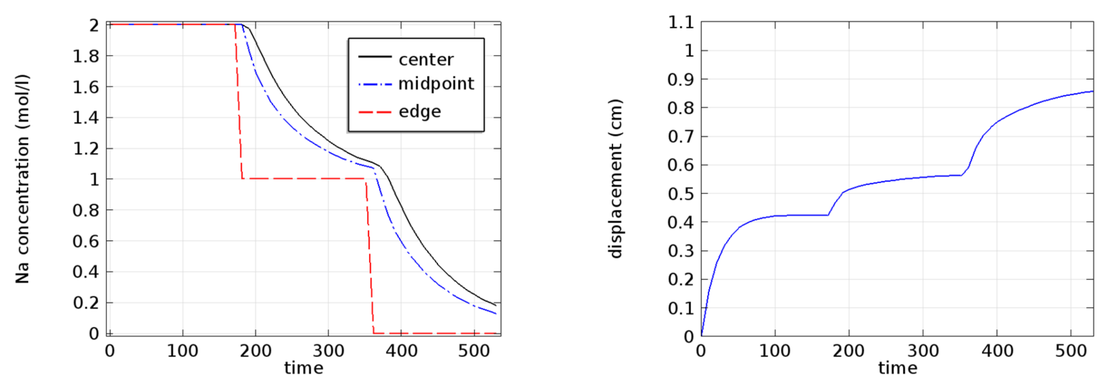

Figure 3. Results from the weakly coupled simulation. The sample swells when it is free from confinement (t<180 d) and when the salinity at the edges is lowered in two steps (from 2 to 1 mol/l during 180 d<t<360 d and from 1 to 0 mol/l during t>360 d).

Conclusions

A large deformation model needed to describe the swelling of bentonite has been developed. The emphasis has been on the rather complicated conceptual and mathematical formulation of the model. With the model, for example, the swelling of saturated bentonite can be simulated when the boundary conditions for a bentonite body are altered (opening of a confined space) and when the salinity of bentonite decreases.

Refenrences

Pulkkanen, V.-M. (to be published in 2016) Doctoral Thesis.

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