PEBS Newsletter No. 6

Model simulations form an integral part of the PEBS. They comprise coupled hydro-mechanical (HM), thermo-hydro-mechanical (THM) and thermo-hydro-mechanical-chemical (THMC) simulations of the various experiments performed in PEBS, and of some earlier experiments. This newsletter presents an overview of a few of the modelling activities performed in PEBS.

THM modelling of the HE-E experiment

The HE-E experiment (Figure 1), a 1:2 scale heating experiment performed at the Mont Terri Rock Laboratory, was set up in the first half of 2011, with start-up of heating in June 2011. The maximum temperature of 140°C was reached in June 2012. The experiment serves to investigate the early post-closure thermal behaviour of the buffer.

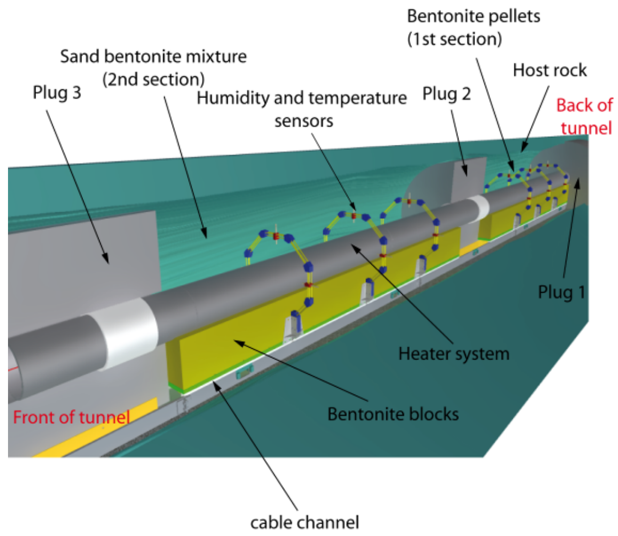

Figure 1. Overview of the Mont Terri HE-E experiment.

The early post-closure phase of a repository is characterised by high temperature gradients and low saturation, and is likely to influence the further development of the canister-buffer-rock system. A profound understanding of the relevant THM processes is thus necessary to assess this development. The respective modelling work is divided into different phases:

- Scoping calculations: These were performed during the planning phase of the experiment, in order to make sure that the experiment layout would meet the requirements regarding temperature development, and that the instrumentation would be adequate.
- Interpretation modelling: This is performed in prediction-evaluation cycles. First predictive calculations are currently being compared to the data measured so far (Figures 2 and 3). A second cycle is in preparation and will be validated against the measurements towards the end of the experiment. In comparison to the scoping calculations, the interpretation modelling goes into more depth, because it can use both the in-situ measured data and also results from parallel laboratory testing to determine material behaviour and parameters.
- Long-term extrapolation: The models and parameters validated and calibrated in the prediction-evaluation cycles will be used for long-term extrapolation up to a state of final saturation and negligible temperature gradients in the buffer.

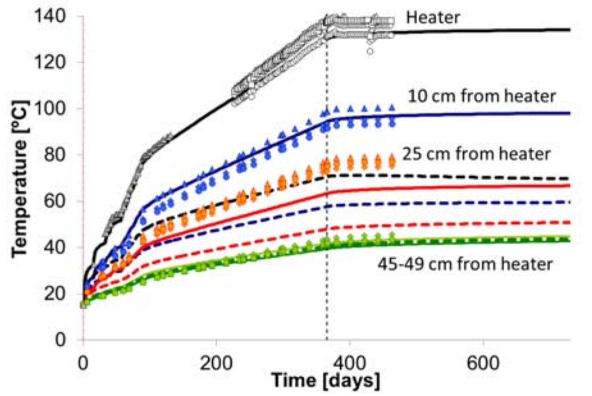

Figure 2. Measured (dots) and calculated (lines) HE-E temperature developments; results from CIMNE's axisymmetric THM coupled model. The dotted lines are results from the first scoping calculation.

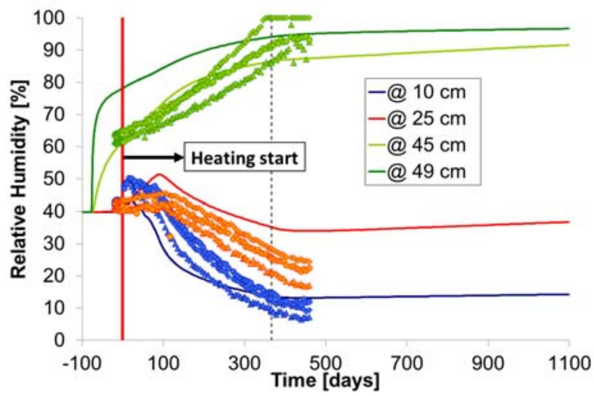

Figure 3. Measured (dots) and calculated (lines) relative humidity development in the bentonite buffer (CIMNE).

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THMC models of heating and hydration corrosion tests

Heating and hydration corrosion lab tests performed at the CIEMAT facilities in Spain on samples of compacted FEBEX bentonite were modelled with the THMC computer code INVERSE-FADES-CORE. Tests included the SC test (2.5 cm long) and the FB3 test (10 cm long), both performed on cylindrical samples of compacted bentonite (Figure 4). Bentonite samples were hydrated from one side at a prescribed liquid pressure while they were in contact with iron powder at 100ºC on the other side.

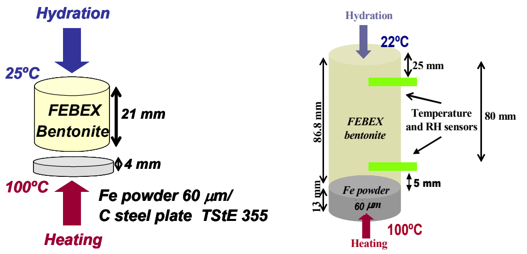

Figure 4. Small (left) and intermediate-scale (right) heating and hydration lab tests to study the interactions of bentonite and corrosion products (Turrero et al., 2011).

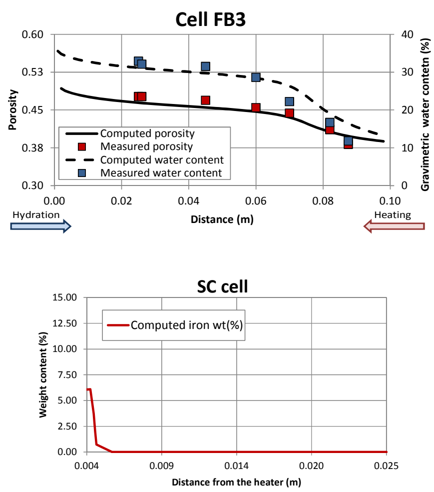

Figure 5. Measured (symbols) and computed (lines) gravimetric water content and porosity in the FB3 test (top) and precipitated Fe in the SC test (bottom).

The tests were modelled with 1D finite element grids. Hydrodynamic, thermal and solute transport parameters were calibrated from previous heating and hydration tests without corrosion products (Zheng et al., 2010). The chemical system is defined in terms of the following primary species: H_2O, H^+, Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-, SO_4^{2-}, HCO_3^- and $SiO_2(aq)$. The models account for homogeneous reactions and heterogeneous reactions such as mineral dissolution/precipitation of calcite, gypsum/anhydrite, quartz and Fe minerals; cation exchange of Ca^{2+}, Mg^{2+}, Na^+, K^+ and Fe^{2+}; and surface complexation using three types of protolysis sites. Iron corrosion is modelled with a constant corrosion rate. The model reproduced the measured gravimetric water content, porosity and temperature at the end of the FB3 test and the measured total precipitated Fe in the SC test (Figure 5).

Long-term extrapolation

The objectives of this task are to extrapolate the data and improved models from the other modelling tasks to the long-term evolution of the repository, and to investigate model uncertainty and its impact on long-term predictions, thus providing input to PEBS Work Package 4. PEBS Work Package 1 involved compiling important processes possibly exhibiting uncertainty in their formulation, as identified by the various national programmes. In order to define the modelling cases for the extrapolation exercise, the processes were evaluated based on these criteria:

- The processes which exhibit uncertainties that have an impact on safety are the most suitable candidates for extrapolation.
- Substantial data to improve their description should be provided by PEBS.
- The modelling cases to be considered should be of general interest (i.e. of interest to more than just one PEBS partner).

These processes and modelling cases were identified:

1. Water uptake in the buffer at temperatures below 100 °C: This case involves modelling of the FEBEX in-situ experiment and comprises the variants of isothermal saturation, long-term heating with a constant temperature of 100°C, and long-term extrapolation using a realistic thermal source term.
2. Thermal evolution of the buffer at temperatures above 100 °C: This is a long-term extrapolation of the Mont Terri HE-E using the real thermal source term.
3. Hydro-mechanical evolution of the buffer deals with the uncertainty in HM evolution of the buffer (pellets), the impact of increased temperature or other factors coupled to heat on the HM properties, and the hydro-mechanical impact from corrosion processes (with feedback from Case 4).
4. Geochemical evolution, especially at the interfaces, involves long-term THMC coupled modelling of canister/bentonite interfaces and concrete/bentonite interfaces, and the long-term evolution of a repository in granite.

There is currently agreement that the models for the relevant processes do in principle exist. They will be checked against the data from the experiments and used for long-term simulation. Long-term extrapolation will be the major modelling task of the coming year, which will feed directly into Work Package 4, "Analysis of impact on long-term safety and guidance for repository design and construction".

Content of the next Newsletter

The following Newsletter will include the latest results discussed at the 4th annual project meeting.

Detailed information see the PEBS web site:

http://www.pebs-eu.de

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