Evaluation of the Predictive Capability of Coupled Thermo-Hydro-Mechanical Models for a Heated Bentonite/Clay System (HE-E) in the Mont Terri Rock Laboratory

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Abstract: Process understanding and parameter identification using numerical methods based on experimental findings are a key aspect of the international cooperative project DECOVALEX. Comparing the predictions from numerical models against experimental results increases confidence in the site selection and site evaluation process for a radioactive waste repository in deep geological formations. In the present phase of the project, DECOVALEX-2015, eight research teams have developed and applied models for simulating an in-situ heater experiment HE-E in the Opalinus Clay in the Mont Terri Rock Laboratory in Switzerland. The modelling task was divided into two study stages, related to prediction and interpretation of the experiment. A blind prediction of the HE-E experiment was performed based on calibrated parameter values for both the Opalinus Clay, that were based on the modelling of another in-situ experiment (HE-D), and modelling of laboratory column experiments on MX80 granular bentonite and a sand/bentonite mixture .. After publication of the experimental data, additional coupling functions were analysed and considered in the different models. Moreover, parameter values were varied to interpret the measured temperature, relative humidity and pore pressure evolution. The analysis of the predictive and interpretative results reveals the current state of understanding and predictability of coupled THM behaviours associated with geologic nuclear waste disposal in clay formations..

1. Introduction

Claystone is being investigated in many countries as a potential host rock for the final disposal of high-level radioactive waste (HLW). Two types of clay, ductile clay (e.g. the Opalinus Clay in Switzerland and Callovo-Oxfordian Clay in France), and plastic clay (e.g. the Boom Clay in Belgium) are being studied intensively in underground laboratories by the international research community. As a geotechnical barrier, bentonite and sand/bentonite mixtures are regarded as favourable materials in most multi-barrier concepts because of their low hydraulic conductivity and high sorption properties. Since both claystone and bentonite are initially water-saturated or partially saturated, the heat emitted by HLW can induce significant changes in the hydro-mechanical properties of such materials.

A series of in-situ heater experiments are being conducted in underground laboratories in argillaceous rock. Worthy of special mention are two full-scale tests, the FE (Full-scale emplacement) experiment in the Mont Terri Rock Laboratory in Switzerland (Müller et. al, 2012) and the Full-scale HA heater tests in the Meuse/Haute-Marne Underground Research Laboratory at the Bure site in France (Armand, 2015). Several preliminary tests have also been carried out, e.g. borehole-scale HE-D and mini-tunnel scale HE-E experiments in the Opalinus Clay in the Mont Terri Rock Laboratory and the TER experiment in the Callovo-Oxfordian (COX) Clay at the Bure site (Wileveau and Su, 2007). Numerous experimental data are available for process understanding, model development and parameter estimation for the complex coupled processes, including:

- A high heater temperature inducing desaturation close to the heater
- Heat transfer occurring in a partially saturated bentonite/clay system
- Desaturation leading to shrinkage deformation of the bentonite, which may generate local micro-fissures with high permeability that are re-sealed due to swelling during the later resaturation process
- High temperatures changing the pore pressure state due to fluid thermal expansion in the surrounding low permeability clay rock.

Numerical tools are often developed to interpret the experimental data. Within the international cooperative project DECOVALEX (DEvelopment of COupled models and their VALidation against Experiments www.decovalex.org), numerical methods and codes dealing with coupled thermo-hydro-mechanical and also chemical processes are continuously being developed (Jing et al., 1995). In the last phase of the DECOVALEX-2015 project, five tasks were analysed, three relating to thermal, hydraulic and mechanical processes in the clay formation and two relating to flow and transport in the fractured rock. One important task is Task B1, in which (1) one borehole heater experiment (HE-D) was studied to understand THM processes in the Opalinus Clay (Garitte et al., 2016), (2) two laboratory column tests were studied to determine THM properties of the buffer materials (bentonite and sand/bentonite mixture), and (3) a half-scale in situ heater experiment(HE-E), involving both host rock and clay buffers exposed to heat (Graupner et al., 2016). The focus of this task was on the modelling of the HE-E experiment (Gaus et al., 2014a), that has been ongoing since 2011. Eight modelling teams from seven countries (Canada, China, Germany, Japan, Korea, Switzerland and the United States) were involved in Task B1. Seven different thermo-hydro-mechanical codes were used to simulate the response of the Opalinus Clay and the buffer materials (a granulated bentonite mixture, bentonite blocks and a sand/bentonite mixture) to thermal loading.

The aims of Task B1 were:

- Verifying the capability of different codes to predict the in situ THM response of a buffer material and surrounding Opalinus Clay to thermal loading on the basis of calibrations performed on small-scale laboratory tests involving backfill material only and an in-situ experiment involving Opalinus Clay only
- Performing interpretative modelling of the HE-E in situ test to estimate parameter sensitivity and to improve conceptual models
- Performing long-term predictions using different codes and conceptual models validated in the early phase of the experiment to estimate a potential time range for full buffer saturation.

Based on the modelling results and estimated parameter values for the Opalinus Clay and the buffer materials from the HE-D experiment and the CIEMAT column tests, predictions were made by all teams before the experimental data were published by the task leader (Garitte, 2016). Interpretation of the measured temperature and relative humidity mainly in the buffer material, as well as the pore water pressure in the clay rock, was conducted.. Finally, long-term predictions focusing on the time for full resaturation of the backfill material were carried out to estimate the experiment duration.

The model predictions and interpretations conducted related to the HE-E experiment allowed the predictive capability of numerical codes for coupled thermo-hydro-mechanical processes in the heated bentonite/clay system to be evaluated. In principle, a prediction does not have to be an exact forecast of the measured value, but may be an estimate of the behaviour of a complex system. As a result, almost all the models were able to reproduce the temperature evolution both in the buffer material and in the clay rock, which indicates that the main thermal processes, even back-coupled with hydraulic processes, can be well understood, at least in the short-term. On the other hand, hydraulic processes react more sensitively and some models could predict reasonable trends and improve their quality by introducing additional coupling functions. Mechanical responses were not analysed in the HE-E experiment because there were no experimental data available for the backfill material.

2. In-situ HE-E heater test

The Mont Terri Rock Laboratory is located in the Opalinus Clay of the Folded Jura Mountains in north-west Switzerland (Fig. 1). The Opalinus Clay is a stiff layered Mesozoic clay of marine origin. Its layered structure results in cross-anisotropic properties, oriented according to the sedimentation plane (bedding plane). The two in-situ experiments (HE-D and HE-E) studied in Task B1 were performed in the Gallery 98 (Fig. 2). At the location of the two in-situ experiments, the bedding plane dips at approximately 45°.

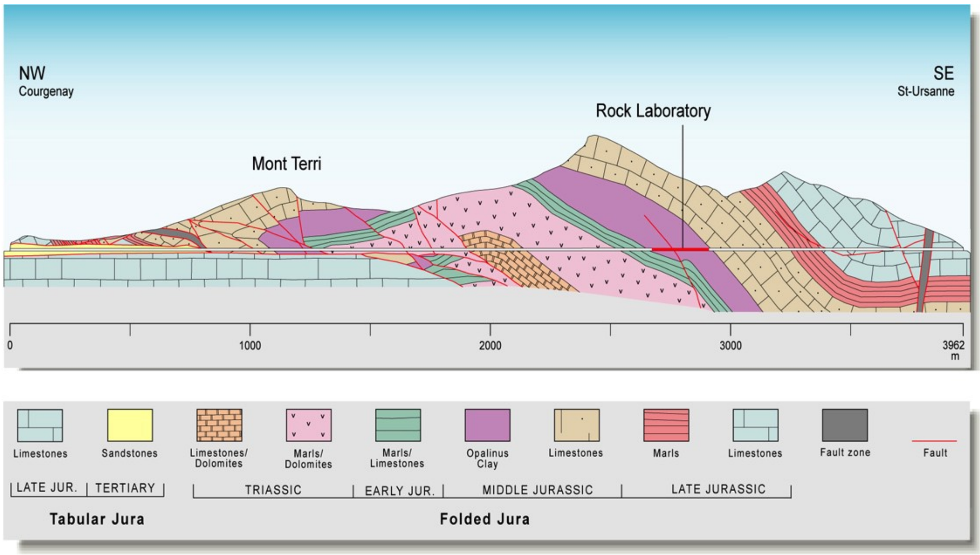

Figure 1: **Geological profile of Mont Teri Jura (Thury & Bossart, 1999).**

The in-situ HE-E experiment is located in the micro-tunnel used for the VE experiment; the experiment was conducted between June 2003 and May 2004 focusing on the changes in the hydro-mechanical properties of the Opalinus Clay due to ventilation effects (Mayor et al., 2005). The micro-tunnel, with a total length of 50 m and a diameter of 1.3 m, was excavated in 1999, twelve years before the HE-E experiment started. This fact led to speculation that a large desaturated zone may exist around the micro-tunnel due to the long open phase, which would determine the initial hydraulic conditions for the HE-E modelling. On the other hand, investigations from the VE experiment showed a very limited excavation damaged zone from a mechanical point of view, even if the micro-tunnel is unlined.

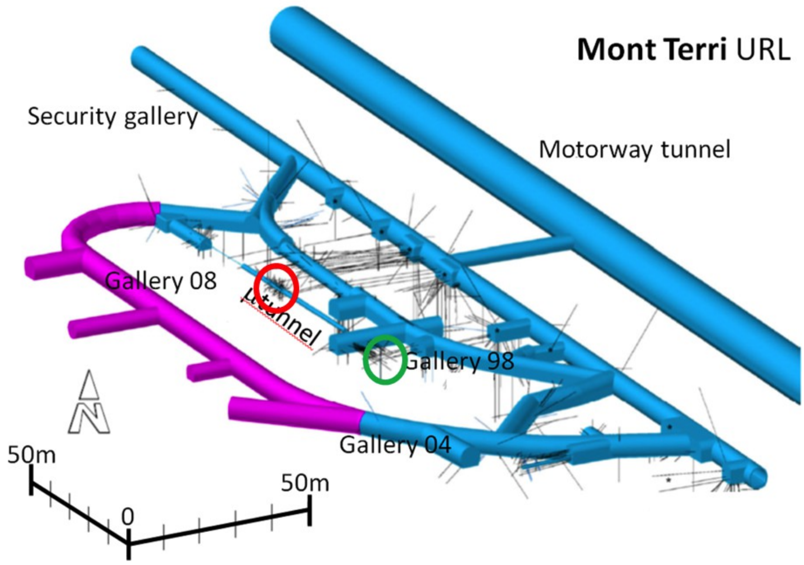

Figure 2: **Location of the two in situ experiments analysed in this work in the Mont Terri Rock Laboratory (green circle: HE-D; red circle: HE-E) (Cite?).**

In a 10 m long section of the micro-tunnel, two heaters with a length of 4 m and an external diameter of 30 cm each were heated independently. They are separated by three concrete plugs with a low thermal conductivity

(Fig. 3). Each heater is wrapped with resistive wires around a tube centralised in a metallic liner. The liner was centred in the tunnel and supported by MX80 bentonite blocks. As backfill material, a sand/bentonite mixture (65/35) was used in one section and granulated MX80 pellets in another section.

No artificial saturation measures were designed or implemented. The bentonite blocks, heaters and buffer instrumentation were emplaced in modules via a rail system that had already been installed in the previous VE experiment. The buffer materials were emplaced using a screw feeder system, resulting in the emplacement properties described in Table 1.

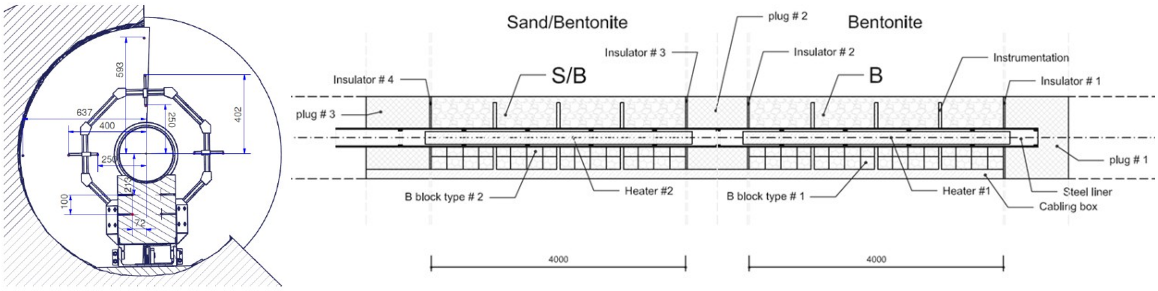

Figure 3: Layout of one heated section of the HE-E experiment (left) and longitudinal section with the micro-tunnel entrance on the left side (right), dimensions in mm (Gaus, ?).

Table 1: "As-emplaced" initial conditions of the HE-E buffer materials.

	Granulated bentonite mixture (GBM) section	Sand/bentonite mixture (S/B) section
Dry density (kg/m^3)	1457	1448
Bulk density (kg/m^3)	1543	1500
Grain density (kg/m^3)	2700	2700
Porosity (-)	0.4604	0.4637
Water content (-)	0.0590	0.0360
Degree of saturation (-)	0.1868	0.1124

All instrumentation was installed before heating started and they were arranged in such a way as to obtain the maximum relevant data density, focusing on thermo-hydraulic responses in the buffer material and rock mass. It consists of:

- Temperature sensors in and on the heater to assist power control
- Numerous thermocouples in the bentonite blocks, Granulated bentonite mixture (GBM) and sand/bentonite mixture (S/B)
- Relative humidity sensors associated with temperature sensors in the buffer (at about 72 locations)
- Relative humidity sensors associated with temperature sensors in the near-field rock mass (at about 20 locations)
- Eight 2-metre long extensometers in the rock
- Piezometers associated with temperature sensors in the rock mass (at about 40 locations).

The instrumentation in the Opalinus Clay is from the VE experiment. In this paper, the focus is solely on sensors located in the middle section of the heater installed in the B section. Generally, the measurements in the GBM (temperature and relative humidity sensors) show a very consistent and redundant pattern. Hence, focusing on only a few sensors is representative of the general behaviour. The high temperature gradient in the GBM and the low temperature gradient in the Opalinus Clay associated with a relatively low and a relatively high thermal conductivity, respectively, can be clearly identified. The processes observed in the column tests (relative humidity patterns characteristic of water redistribution between hot and cold zones) and in the HE-D experiment (pore water pressure response to thermal pulse) can be clearly identified in the HE-E experiment.

Prior to the HE-E experiment, the initial temperature in the host rock was approximately 15°C. During the first year of the experiment, the power was increased in the two heaters in order to reach the target heater temperature (140°C) after one year (Figure 4). To do this, a slightly higher power was required in the GBM section, indicating that this material has a slightly higher thermal conductivity than the S/B mixture. After the first year, the power was modulated to maintain a constant heating temperature. The analysis of the buffer temperature measurements shows that a steady-state is quickly reached in the buffer and hence the entire heat flux produced by the heaters is transmitted entirely to the Opalinus Clay.

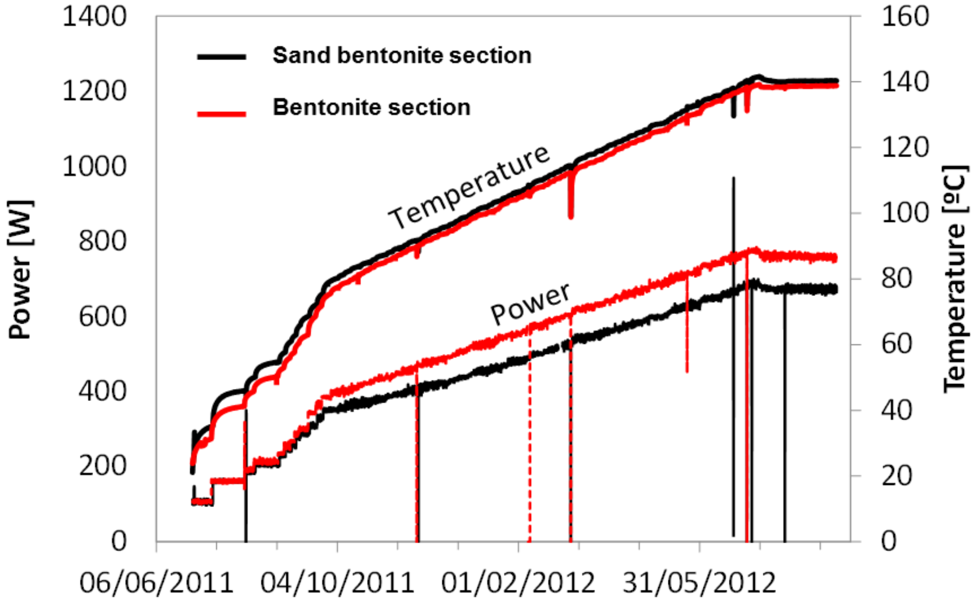

Figure 4: **Applied power in each of the HE-E heaters and resulting heater surface temperature.**

3. Modelling approaches

3.1 THM processes involved in the HE-E experiment

Both the Opalinus Clay and the buffer are considered as fully and partially water-saturated porous media, respectively. When such materials are subjected to thermal loading, the following processes may occur:

- Temperature increase at the heater surface leads to heat transfer from the heater by thermal conduction and convection in the system
- Drying and desaturation along with possible shrinkage may occur in the buffer material closer to the heater
- Vapour may diffuse toward and condense at the low temperature zone near the rock-buffer interface
- Change in saturation due to drying can strongly alter the thermal conductivity and thereby significantly affect the heat conduction, especially in the buffer material.
- Temperature increase results in thermal expansion of both solid matrix and pore water. Pore pressure will increase especially in the Opalinus Clay because of the higher thermal expansion coefficient of water in comparison with the solid matrix and the low permeability of the clay rock
- Increase in pore pressure in the host rock in the vicinity of the heat source results in a hydraulic gradient that triggers water flow away from the heat source and a change in effective stress state, which may influence mechanical deformation behaviour
- Thermally induced deformation may be the dominant mechanical process

3.2 Codes used for HE-E experiment

The complex coupled mechanisms can be analysed by numerical modelling. The governing equations used in the numerical models are based on the conservation of heat, mass and momentum (Garitte et al., 2016). However, different models are used by the individual teams. For example, some teams used the Richards flow model for unsaturated flow simulation and others applied the multiphase flow model also taking gas pressure into consideration. Concerning hydro-mechanical coupling, Biot's effective stress principle is assumed, but the modification for unsaturated flow is realised by two approaches (Eq. 1 and 2):

$$\boldsymbol{\sigma}_{eff} = \boldsymbol{\sigma}_{tot} - \chi p^{w} \mathbf{I}$$
$$\chi = \begin{cases} \alpha, if\ p \geq 0 \\ 0, if\ p < 0 \end{cases} \quad (1)$$

or

$$\boldsymbol{\sigma}_{eff} = \boldsymbol{\sigma}_{tot} - a p^{w} \left(S^{w}\right)^{c} \mathbf{I} \quad (2)$$

where σ_{eff} is the effective stress, σ_{tot} is the total stress vector, χ is Bishop's coefficient, $\boldsymbol{p^w}$ is the pore pressure, $\boldsymbol{S^w}$ is water saturation, and α is the constant model parameter.

Additionally, constitutive relationships that are specific to the material thermal, hydraulic and mechanical behaviour are also assumed according to the experimental data available for the individual materials (Wang et al., 2016). The governing equations, with their corresponding boundary and initial conditions, were numerically solved with different computer codes based on different numerical methods. BGR/UFZ and ENSI modelling teams used the finite element method, with the OpenGeosys computer code (Kolditz et al., 2014). CNSC and JAEA teams also used the finite element method, with the COMSOL and THAMES codes respectively. CAS team used a self-developed numerical code EPCA^{3D}, which is a combination of multiple techniques and theories, such as finite element method, cellular automaton, elasto-plastic theory and principle of statistics etc (Pan et al, 2009a, Pan et al, 2009b, Pan and Feng, 2013).. The CNWRA team used the Finite Difference code FLAC. The KAERI team used the Finite Difference code FLAC3D (Itasca, 2012). The LBNL team used TOUGH-FLAC, based on linking the TOUGH2 multiphase flow simulator (Integral Finite Difference), with the FLAC3D geomechanical code (Finite Difference Method) (Rutqvist et al., 2002; 2014). . The thermal, hydraulic and mechanical anisotropy for Opalinus Clay were considered by most teams, though JAEA and LBNL only considered the thermal anisotropy.

Seven teams developed a 3D THM model and one team (CNWRA) developed a 2D THM model for the HE-E experiment. The various teams employed individual approaches for the modelling sequence of (1) a ventilation period starting in 1999 when the micro-tunnel was raise-bored (horizontally), (2) emplacement of the backfill material 30 days before the start of heating, and finally, (3) the first 3 years of heating from the start of heating on June 30, 2011.

Table 1 summarises the computer codes and associated numerical methods used by each team. The colour code associated with each team indicates the modelling results in the following figures.

Table 1: Colour codes, computer codes and numerical methods used by the teams in task B1

Team & Colour Code	Code	Numerical method
BGR/UFZ	OpenGeoSys	FEM
CAS	EPCA3D	EPCA
LBNL/DOE	TOUGH-FLAC	DFN/FDM
ENSI	OpenGeoSys	FEM
CNSC/IRSN	COMSOL	FEM
JAEA	THAMES	FEM
KAERI	FLAC	FDM
CNWRA/NRC	xFlo-FLAC	FDM

List of abbreviations:

- BGR: Federal Institute for Geosciences and Natural Resources
- UFZ: Helmholtz Centre for Environmental Research
- CAS: State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences
- LBNL: Lawrence Berkeley National Laboratory
- DOE: Department of Energy

- ENSI: Swiss Federal Nuclear Safety Inspectorate
- CNSC: Canadian Nuclear Safety Commission
- IRSN: French Institute for Radiological Protection and Nuclear Safety
- JAEA: Japan Atomic Energy Agency
- KAERI: Korea Atomic Energy Research Institute
- CNWRA: SwRI Center for Nuclear Waste Regulatory Analyses
- NRC: Nuclear Regulatory Commission
- DFN: Discrete Fracture Network.
- FEM: Finite Element Method
- FDM: Finite Difference Method
- EPCA: Elasto-Plastic Cellular Automaton Method

All components with different physical properties, including the Opalinus Clay, bentonite blocks, granulated bentonite mixture (GBM), sand/bentonite mixture (S/B) concrete plugs and heaters, were considered in the numerical models. Different realisations, e.g. structured grid and unstructured mesh, half domain and full domain, were performed by different teams. Three examples are illustrated in Figure 5.

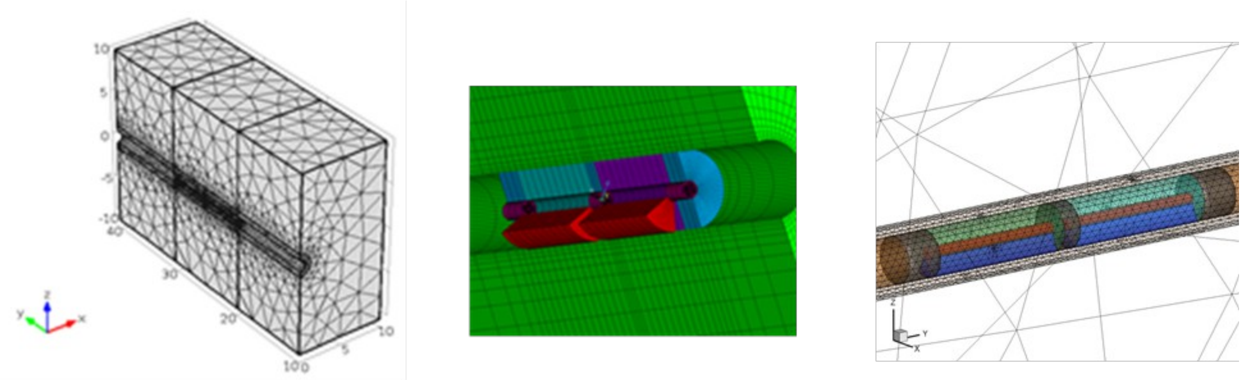

Figure 5: HE-E model: CNSC (l), CAS (m) and BGR (r).

3.3 Model conditions and parameters

As already stated, the teams used calibrated parameters from their two previous numerical simulations of the Opalinus Clay (HE-D) and buffer materials (column tests) in Task B1. Therefore, the parameters used for modelling the HE-E experiment are slightly different for individual modelling teams (Tab. 2).

Table 2: Main Opalinus Clay parameters considered by the teams

		BGR/UFZ	CAS	CNSC	CNWRA	ENSI	JAEA	KAERI	LBNL
Young's modulus in the bedding plane [MPa]	E_h	9300	10000	8000	7000	10000	6000	10000	5000
Anisotropy ratio	E_h/E_v	1.6	2.5	2.7	1.0	2.5	1.0	2.5	1.0
Poisson's ratio [-]	ν_{hh}	0.33	0.24	0.29	0.27	0.24	0.27	0.24	0.3
	ν_{vh}	0.38482	0.33	0.33	-	0.33	-	0.33	-
Shear modulus [MPa]	G_{vh}	2338.71	1200	1000	2756.0	1613.0	-	1200.0	1920.0
Cohesion [MPa]	c'								2.2-5
Friction angle [°]	φ								23-25
Biot [-]	b	0.6	0.6	0.75	-	0.0	0.6		0.6

		BGR/UFZ	CAS	CNSC	CNWRA	ENSI	JAEA	KAERI	LBNL
Porosity	**φ**	**0.137**	**0.137**	**0.12**	**0.137**	**0.2**	**0.157**	**0.157**	**0.15**
Solid grain density [kg/m³]		**2500**	**2340**	**2700**	**2450**	**2740**	**2450**	**2450**	**2700**
Intrinsic permeability [m²] (α is the anis. ratio)	$k_{//}$	**2.E-19**	**1.E-19**	**2.5E-20**	**5.E-20**	**2.E-20**	**1.E-20**	**1.E-19**	**5.E-20**
	k_{per}	**2.E-20**	**5.E-20**	**1.E-20**	**5.E-20**	**4.E-21**	**-**	**5.E-20**	**5.E-20**
	k_0^{*2}	**1E-19**	**8.E-20**	**3.E-20**	**5.E-20**	**1.E-20**	**-**	**8.E-20**	**5.E-20**
	α_k^*	**10**	**2**	**4**	**1**	**5**	**-**	**2**	**1**
Thermal conductivity [W/(mK)]	$\lambda_{//}$	**2.15**	**2.15**	**2.15**	**1.77**	**2.15**	**-**	**2.15**	**2.15**
	λ_{per}	**1.2**	**1.19**	**1.19**	**1.77**	**1.19**	**-**	**1.19**	**1.19**
	λ_0^*	**1.77**	**1.77**	**1.77**	**1.77**	**1.77**	**2.15**	**1.77**	**1.77**
	α_λ^*	**1.79**	**1.79**	**1.79**	**1**	**1.79**	**-**	**1.79**	**1.79**
Heat capacity of the solid [J/(kgK)]	C_s	**995**	**995**	**946.5**	**1000**	**800**	**800**	**1000**	**900**
Linear solid thermal expansion coefficient E-05 [K-1]	b_s	**1.40**	**1.00**	**1.70**	**1.60**	**2.60**	**2.60**	**2.60**	**1.40**

* Dependent parameters

The initial pore water pressure at the Mont Terri site is measured as approximately 2 MPa. The lower value used by most of the teams reflects the fact that the test location was subject to drainage effects due to the existence of Gallery 98 and Gallery 2008.

Table 3: Thermal and mechanical initial and hydraulic boundary conditions

		BGR/UFZ	CAS	CNSC	CNWRA	ENSI	JAEA	KAERI	LBNL
Model		**3D**	**3D**	**3D**	**2D axisymm.**	**3D**	**3D**	**3D**	**3D**
Couplings		**THM**	**THM**	**THM**	**THM**	**THM**	**THM**	**THM**	**THM**
Total stresses [MPa]	σ_{xx}	5	4.5	4.3	4.28	-	-	4.5	4.5
	σ_{yy}	3	2.5	2.2	4.28	-	-	2.5	2.5
	σ_{zz}	7	6	6.5	-	-	-	6.0	6.5
Water pressure [MPa]	p_w	0.9	0.9	1	0.1-0.9	01-0.978	2	1.5	1.2
Temperature [ºC]	T	15	15	15	15	15	15	15	15

The thermal, hydraulic and mechanical boundary conditions are defined on the heaters and on the external boundaries. As the thermal load, most teams (....) applied heat fluxes to the heaters, but some of them (....) applied temperature directly.

The constitutive functions which show strongly coupled mechanisms are important for the evaluation of the thermal, hydraulic and mechanical behaviour of buffer material. Based on the laboratory data, the teams used different approximations provided by the calibration of the column tests. Some teams, e.g. CSNC, used the

Brooks-Corey model (Eq. 3) and others, e.g. BGR/UFZ, CAS and LBNL, used the van Genuchten model (Eq. 4) to simulate the retention process. Figure 6 shows the hydraulic properties for a partially water-saturated granulated bentonite and Figure 7 shows the saturation-dependent thermal conductivity for the bentonite pellets and blocks.

$$S_{eff} = (\alpha P^c)^{-n} \tag{3}$$

$$p^c = -p^0 \left[\left(S_{eff} \right)^{-1/m} - 1 \right]^{(1-m)} \tag{4}$$

where S_{eff} is the effective saturation and P^c is the capillary pressure. ***n*, α,** and ***m*** are the parameters in the respective models.

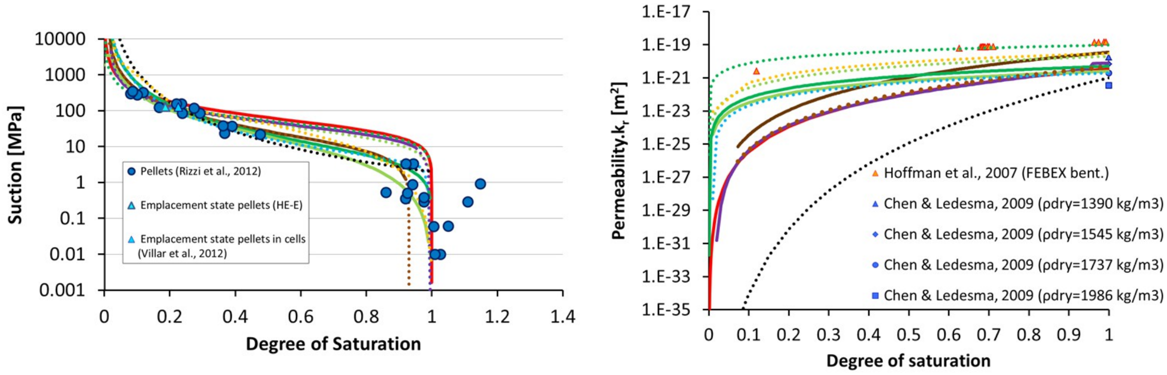

Figure 6: **Retention (l) and relative permeability (r) functions for partially saturated granulated bentonite.**

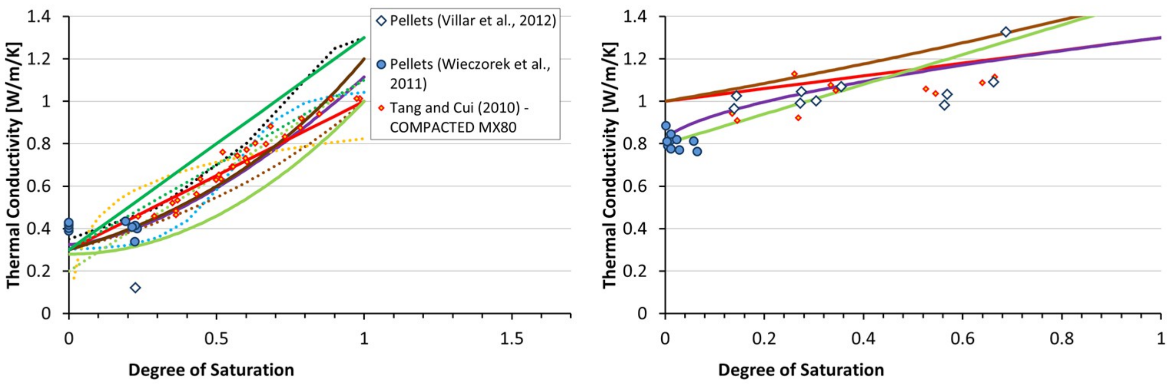

Figure 7: **Relationship between thermal conductivity and water saturation for granulated bentonite (l) and bentonite blocks (r) (data from Wieczorek et al. 2011).**

4. Predictive modelling

As an initial boundary value problem, the initial conditions are important for the solution. Due to a long pre-history before the heating started, the initial conditions, especially the hydraulic and mechanical conditions, may have changed. In order to determine the mechanical and hydraulic initial conditions in the HE-E experiment, the teams have simulated the previous activities in the micro-tunnel, namely tunnel excavation, ventilation opening for 13 years at a constant relative humidity of 98% at the tunnel surface and emplacement of the bentonite buffer and heaters 75 days before start of heating. The simulation of the tunnel being open for 13 years was simplified by most teams by applying a constant suction value of 2.6 MPa (corresponding to a relative humidity of 98%) at the tunnel wall (e.g. LBNL). In reality, the tunnel was exposed to a complex history including ventilation experiments, and the average 98% relative humidity was inferred from information in Gaus et al. (2014). This pre-history simulation creates a pressure sink around the tunnel with a slight desaturation of the near-field rock, if no excavation damaged zone around the tunnel is considered.

The predictive modelling exercise was done using the parameters calibrated in the previous work. The parameters for the Opalinus Clay were taken from the modelling of the HE-D experiment (Garitte et al., 2016) and for the buffer material from the column tests (Graupner et al., 2016). A systematic analysis was performed by comparing all predicted results from the teams and measured data. With the focus on the thermal and hydraulic behaviour of the bentonite buffer material, data at the selected sensors are presented in this paper.

Figure 8 shows measured and modelled temperature distribution along two vertical profiles above and below the heater after 545 days of heating. The profile below the heater passes through the compacted bentonite blocks (modelling results: dashed lines, and measurements: white and red circles). The profile above the heater passes through the GBM backfill (calculations: solid lines, and measurements: squares). The predicted temperature in the rock (distance > 0.5 m) provided by three teams (BGR/UFZ, CAS and CNWRA) fits quite well to the measurements. The predicted temperature in the granulated bentonite mixture is slightly underestimated and the modelled temperature in the bentonite blocks is overestimated. The overestimated temperature in the blocks is affected by uncertainties and lack of data on the thermal conductivity of the bentonite blocks. With some exceptions, these phenomena of slight under- and over-estimation of temperature can also be observed in Figures 9 to 11, which include modelling predictions of all eight modelling teams. Nevertheless, most measured trends are reproduced very satisfactorily. The wide range of predicted temperatures from different models is solely due to the thermal conductivity used, which is again influenced by the hydraulic process.

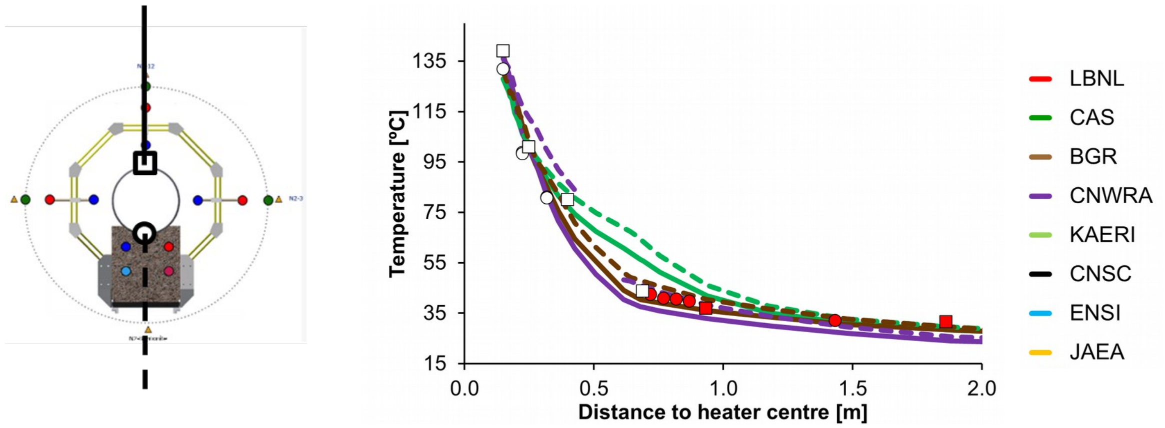

Figure 8: **Vertical measured and modelled radial temperature profiles on 26.12.2012 (0 is the centre of the heater).**

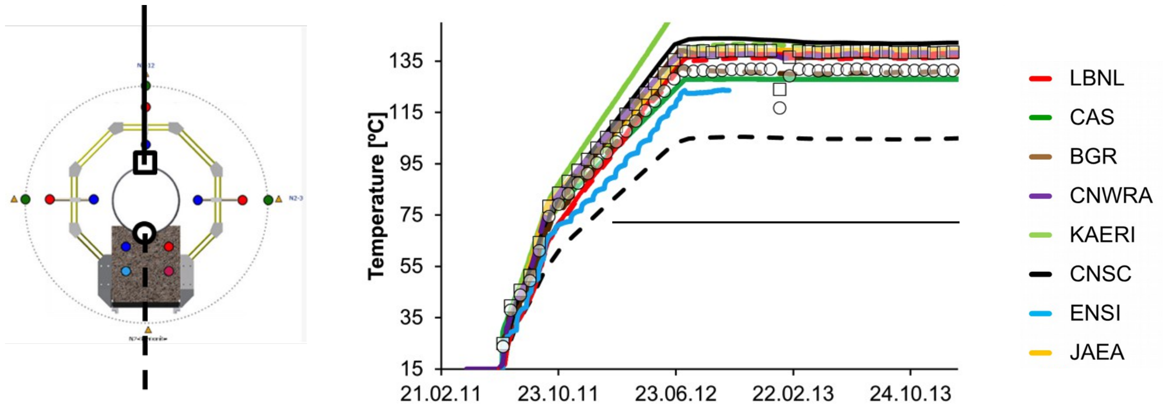

Figure 9: **Measured and predicted temperature evolution at the heater surface.**

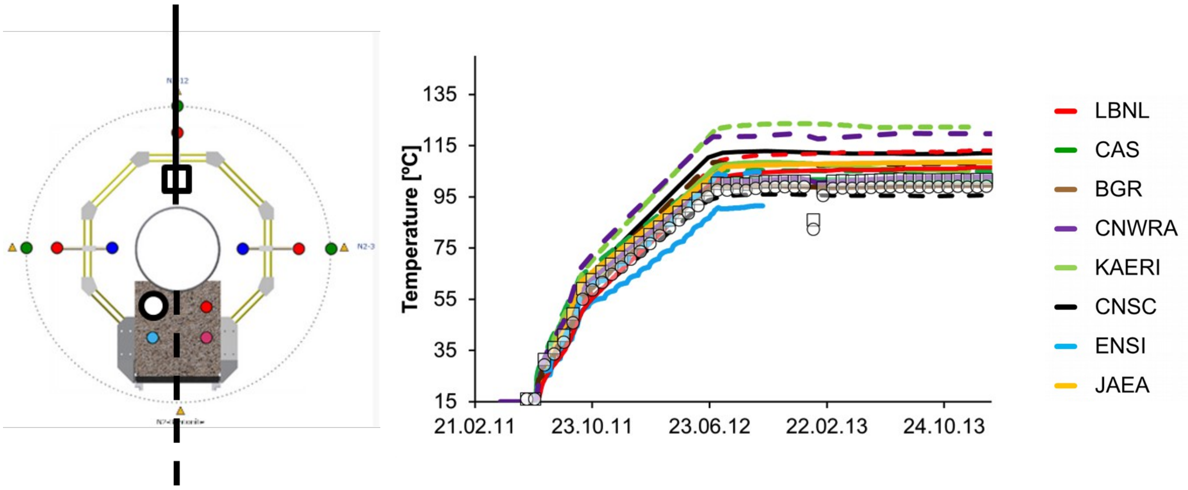

Figure 10: **Measured and predicted temperature evolution at 7 cm and 10 cm from the heater surface in the bentonite blocks and the GBM, respectively.**

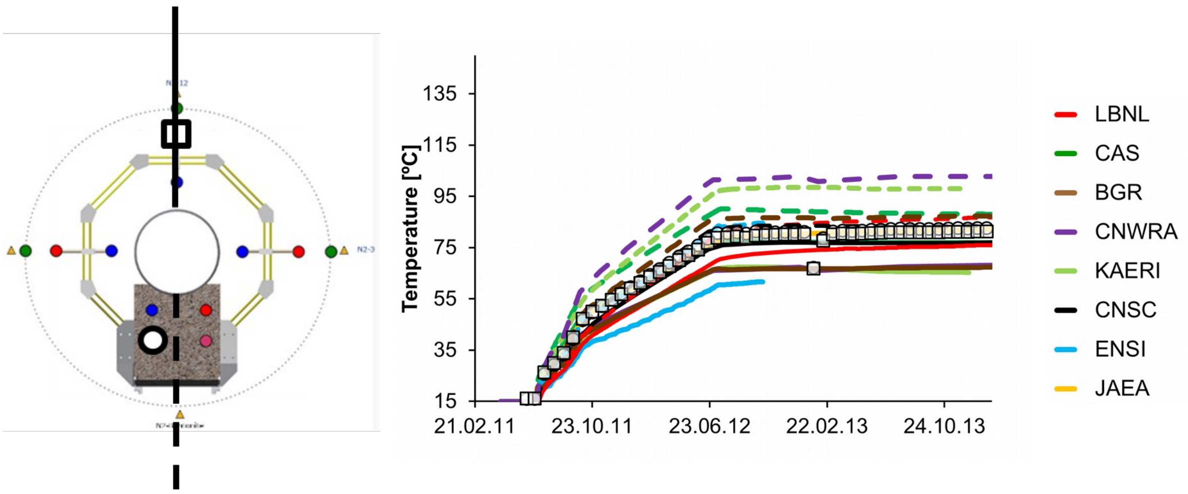

Figure 11: **Measured and predicted temperature evolution at 17 cm and 25 cm from the heater surface in the bentonite blocks and the GBM, respectively.**

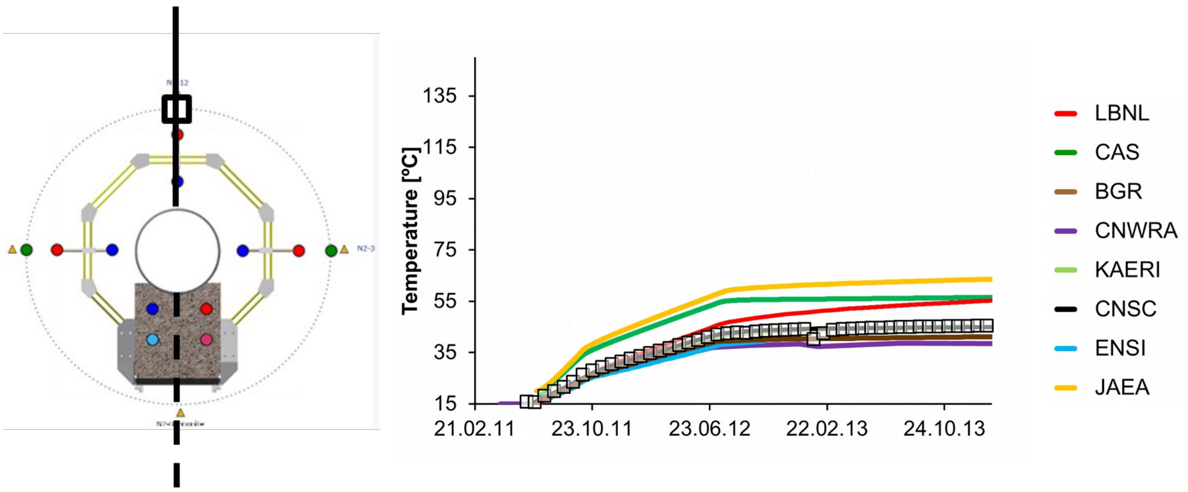

Figure 12: **Measured and predicted temperature evolution on the tunnel surface (54 cm from the heater surface) in the GBM section.**

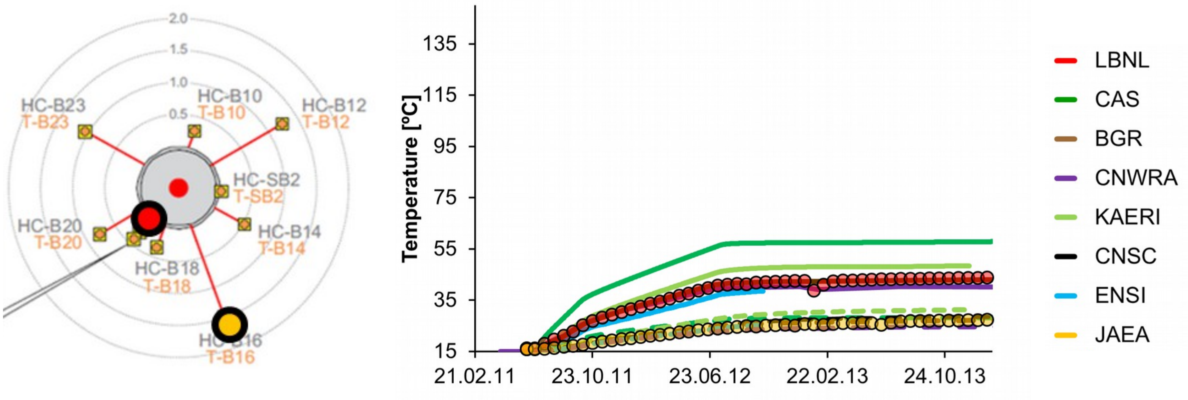

Figure 13: **Measured and predicted temperature evolution at 57 cm and 198 cm from the heater surface in the Opalinus Clay.**

In the Opalinus Clay there are several boreholes equipped with temperature sensors. Observing two sensors, one located close to the tunnel surface and the other about 1.3 m from the tunnel surface, the calculated temperature development agreed quite well with the measurement in both trend and magnitude, even though an isotropic thermal model was used by the CNWRA team (Fig. 13).

Temperature distribution and evolution calculated by heat transport is clearly controlled by thermal conductivity, which due to the saturation-dependent thermal conductivity in the buffer material (Fig. 7) is significantly affected by flow processes in the buffer.. A reasonable reproduction of the saturation state is therefore an important condition for the temperature calculation in the coupled calculations. While the main process in the flow regime could be captured by most teams (Fig. 14 & 15), some teams overestimated the saturation state and, therefore, overestimated the relative humidity as well. The overestimation of the relative humidity thus led to somewhat larger disagreements between the calculated temperature and the measured one (KAERI & CNWRA).

The permeability of clay rock and buffer materials is a key parameter for flow processes. In unsaturated porous media, the relative permeability and retention curve (suction pressure) characterised in the laboratory (Fig. 6) are also very important as these may dominate the flow regime. The retention curve is often difficult to determine experimentally for soil with swelling behaviour.

All models can simulate the temporal evolution of the relative humidity, with an initial increase and decrease thereafter for all sensors in the buffer material due to moisture movement. This phenomena can be described by evaporation and transport of vapour induced by the thermal gradient using vapour diffusion models based on empirical formulas for the atmospheric vapour diffusivity. Some teams overestimated the relative humidity, particularly in the period when the temperature reached the maximum value of 140 °C for the heater (Fig. 14 & 15).

A desaturated zone around the tunnel is observed after 13 years of being open (Fig. 16 & 17). The extent of the desaturated zone is however limited. At the sensor located 1.3 m away from the tunnel surface, the relative humidity is a constant 100 % from the beginning. The granulated bentonite mixture with an initial relative humidity of 40% and the bentonite blocks (50%) take up additional water by inflow from the Opalinus Clay, which results in a reduction of the relative humidity to about 80 % closer to the tunnel surface (Fig. 17). The longer term gradual increase in the relative humidity at these points is due to the water supply from the clay rock on the one hand and, on the other hand, to the migration and condensation of vapour coming from the inner parts of the buffer. This characteristic behaviour was unfortunately not captured. The CAS team made a reasonable prediction of the increase trend, but not the magnitude. In Fig. 16, the shift of RH from unsaturated state to full saturation from July to October, 2012 was well reproduced by CNSC model, which includes a thin layer of EDZ with reduced water retention capacity (40 % in α_w of van Genuchten model) at the inner surface of the tunnel. This may indicate the predominance of the capillary barrier effect induced by the EDZ that is abundant in microcracks, which significantly modulates and reduces water flow from the host rock towards GBM and thus maintains full saturation at later stage.

The initial pore water pressure at the start of heating was not fully captured even if a modelling of the pre-heating period was done. The pore pressure at a distance of 2.47 m from the micro-tunnel centre was subject to atmospheric pressure, which indicated that the sensor is already located in the ED/dZ (excavation damaged or at least disturbed zone). The pore pressure at a distance of 4.87 m from the micro-tunnel centre was measured as 3 bar before the heating, which indicated that the sensor is located in the pressure sink zone. Most teams (BGR/UFZ, CNSC, CNWRA, and LBNL) predicted the initial pressure distribution reasonably well, but with an overestimation. The predicted water pressure response to the thermal pulse is adequate (Fig. 18). The calculated pressure disappeared due to atmospheric pressure conditions set in Gallery 98 by some teams (BGR/UFZ. CNWRA, and LBNL) and the high permeability of clay rock used (BGR/UFZ).

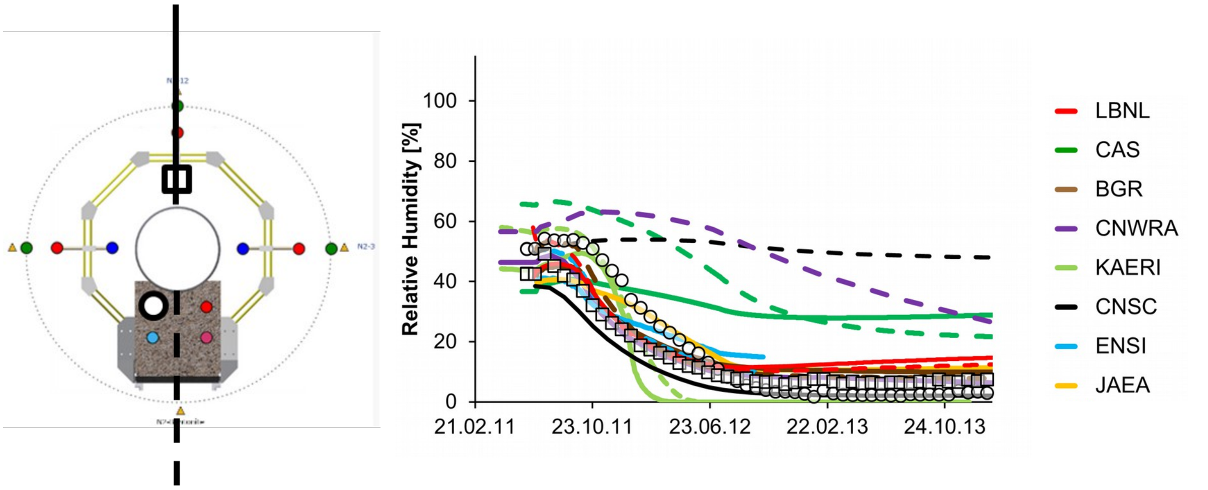

Figure: 14 **Measured and predicted relative humidity evolution at 7 cm and 10 cm from the heater surface in the bentonite blocks and the GBM, respectively.**

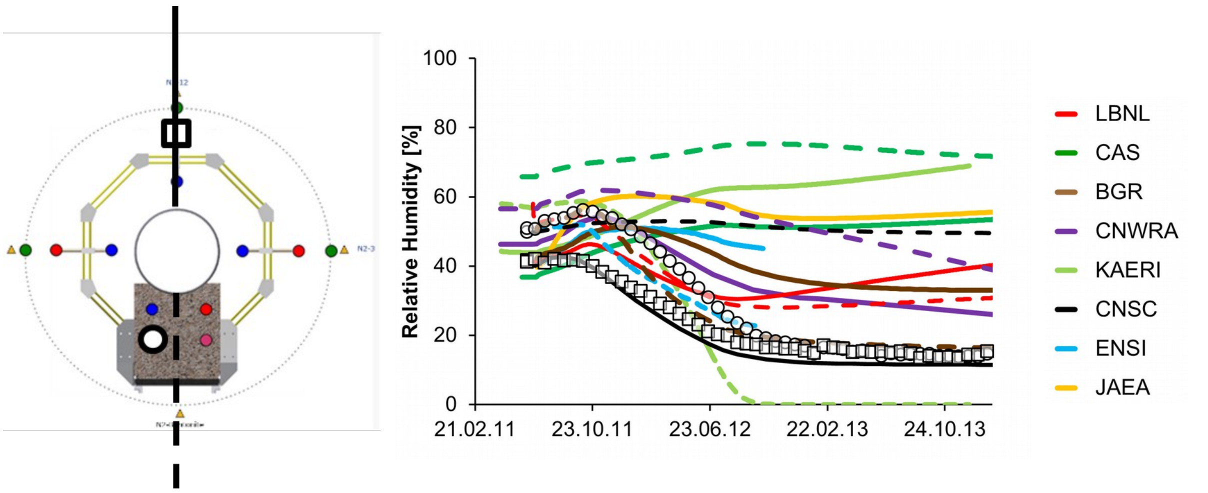

Figure 15: **Measured and predicted relative humidity evolution at 17 cm and 25 cm from the heater surface in the bentonite blocks and the GBM, respectively.**

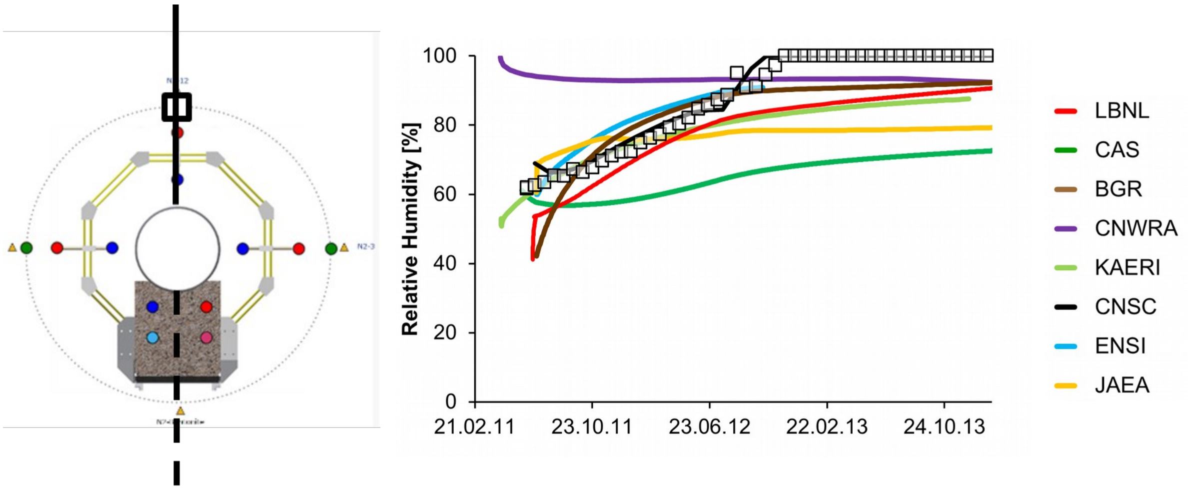

Figure 16: Measured and predicted relative humidity evolution at 54 cm from the heater surface in the GBM.

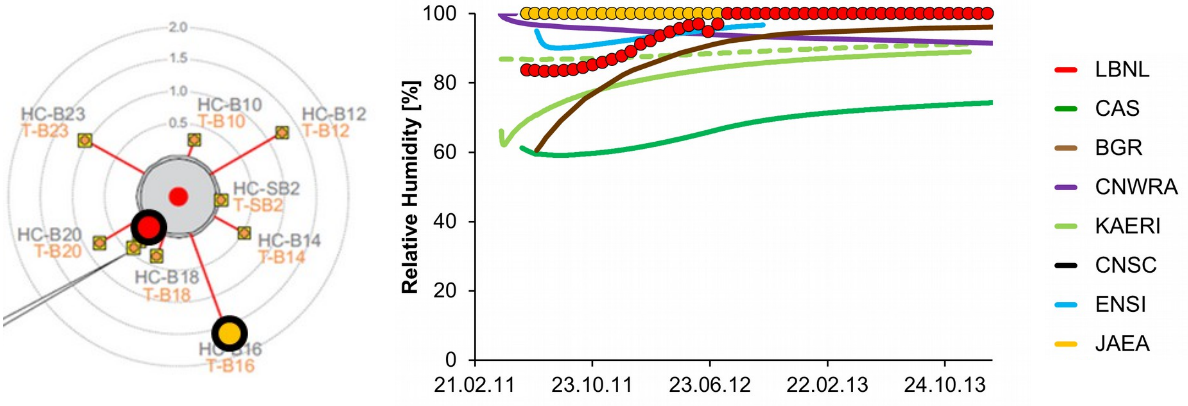

Figure 17: predicted relative humidity evolution at 57 cm and 198 cm from the heater surface Measured and in the Opalinus Clay.

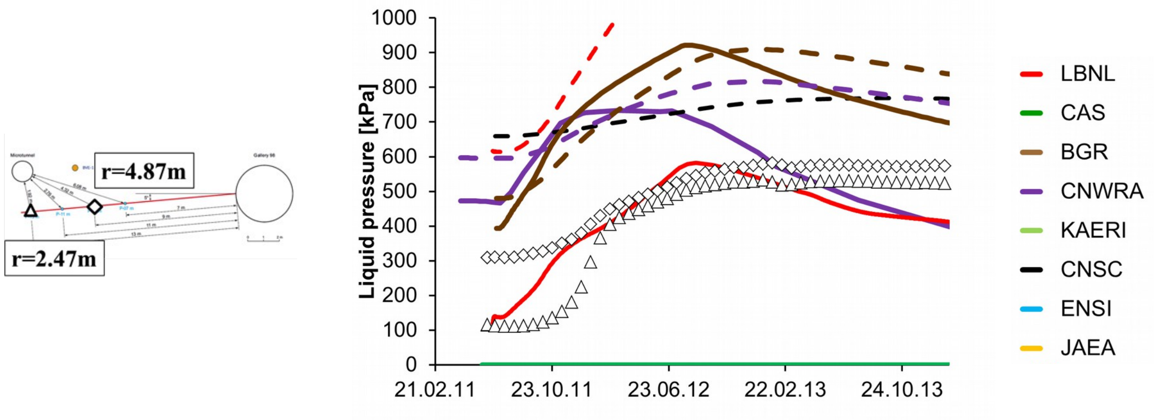

Figure 18: Measured and predicted pore water pressure evolution at 247 cm (full lines) and 487 cm (dashed lines) from the heater surface in the Opalinus Clay.

5. Interpretative modelling

The publication of the experimental data allowed the teams to improve the modelling results from the predictions against the measurements, thus improving the understanding of the coupled thermal-hydraulic and mechanical processes. In the interpretative modelling, all teams applied their model already used in the predictive modelling. Extensive parameter studies were done especially for temperature development in the buffer material. Some teams (BGR/UFZ and LBNL) also implemented additional functions, e.g. temperature-dependent retention behavior under high temperature. This function helped improve the modelling of the relative humidity under high temperature in the column tests (Graupner et al., 2016), but there was no significant improvement for the HE-E experiment.

By varying the thermal conductivity and heat capacity of the buffer material, a much better agreement between the measured and calculated temperature was achieved by all teams. This is obvious in the results of the CNSC and KAERI teams (Fig. 19 versus Fig. 9 and Fig. 20 versus Fig. 11). Particularly the temperature close to the heater can be better matched than the temperature in the granulated bentonite mixture and bentonite blocks because the latter is more dependent on the hydraulic conditions. A wide spectrum of calculated temperatures between 60 and 95°C is still calculated by different teams when the heater is subject to 140 °C (Fig. 20). This difference is not caused by the thermal conductivity but by using different retention curves and relative permeability models.

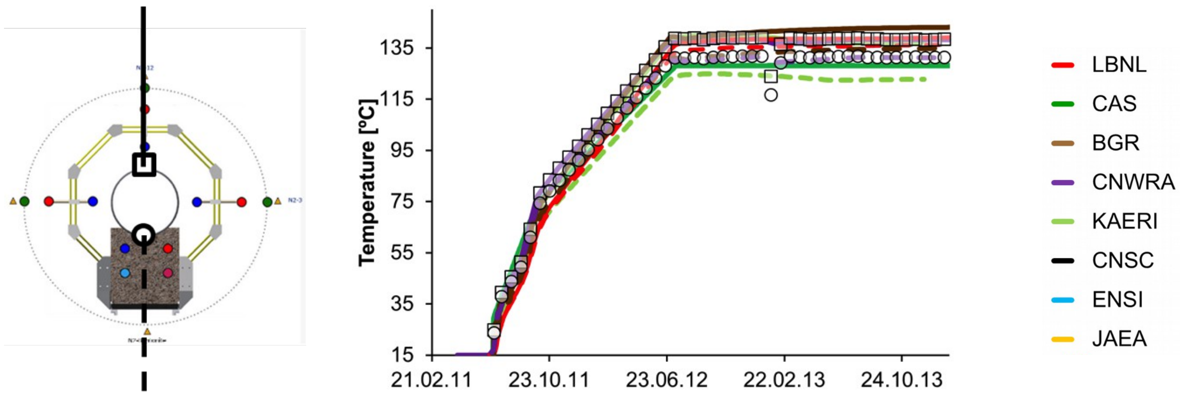

Figure 19: Measured and modelled temperature evolution at the heater surface.

One obvious deviation between predicted results and measurements is the evolution of relative humidity in the buffer. Compared with the predicted relative humidity presented in Figure 15, CAS and CNWRA modelling teams improved their results by using a similar vapour diffusion model as other teams (Fig. 21). However, a much better agreement cannot be achieved even by performing an extensive parameter sensitivity study including buffer intrinsic and relative permeability, diffusion coefficient and water retention curve. The minor improvement (Fig. 22 versus Fig. 16) was simply the result of a slight change in the water retention curve for the bentonite pellets (LBNL). The CNSC team successfully introduced a non-linear vapour diffusivity enhancement factor, which again depends on the water saturation, in the vapour diffusion model.

The analysis done by LBNL confirmed the conclusion that the moisture content in the inner and middle parts of the buffer achieves a pseudo steady-state dictated by two-way diffusion, i.e. thermally driven vapour diffusion and a counter-flow by capillary driven diffusion.

It is therefore obvious that the hydraulic retention curve, relative permeability model and vapour diffusion model dominate the saturation state in the buffer material.

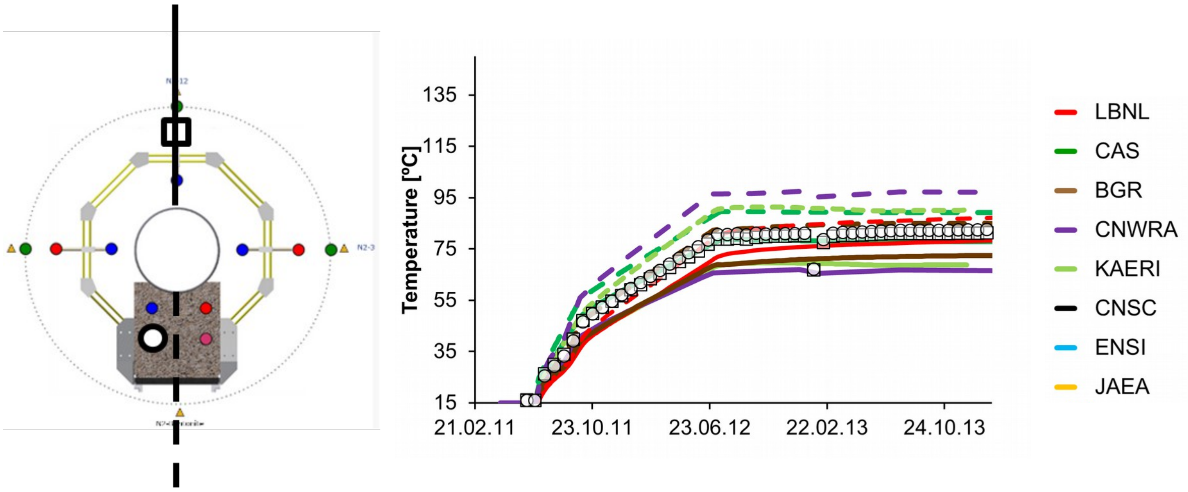

Figure 20: **Measured and modelled temperature evolution at 17 cm and 25 cm from the heater surface in the bentonite blocks and the GBM, respectively.**

An additional material group around the micro-tunnel was introduced to consider the properties of the EDZ caused by tunnel excavation. The BGR/UFZ team assumed that the EDZ has 5-times higher hydraulic conductivity than intact clay rock and an enhanced porosity. Using this model, the initial pore pressure can be well reproduced by modelling years of pre-heating activities. In addition, the entry pressure in the retention curve for the EDZ was also reduced considering the enhanced porosity in the EDZ.

The pore pressure increase was largely due to the thermal expansion of liquid. A gradual decrease should be observed because of the consolidation process. The overestimation of the decrease rate can be found in all model results. The BGR/UFZ team varied the storage coefficient in the hydraulic Richards' flow model. A better agreement with the experimental observations can be obtained when the storage coefficient is doubled from 1E-9 to 2E-9 /m.

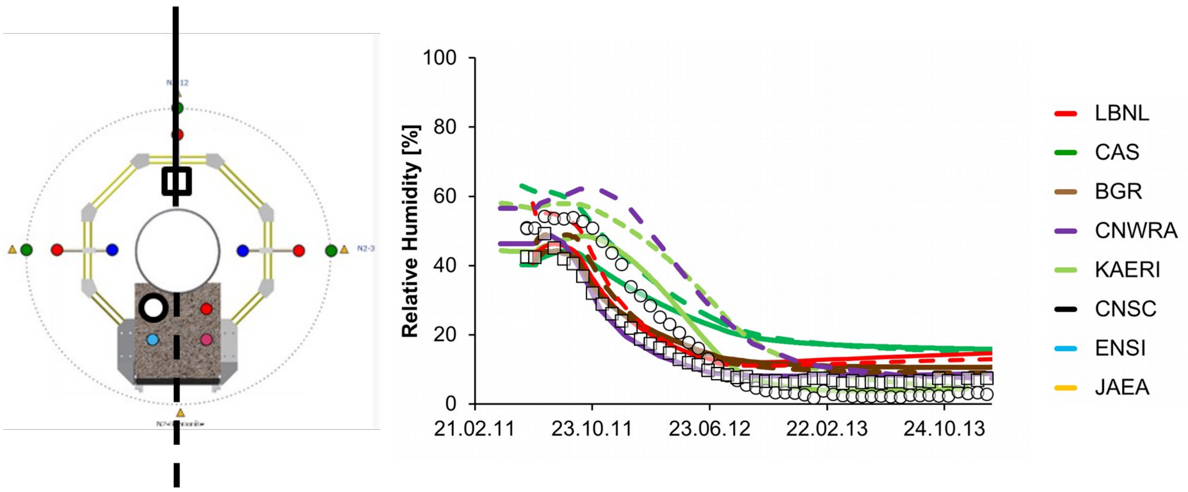

Figure 21: **Measured and modelled relative humidity evolution at 7 cm and 10 cm from the heater surface in the bentonite blocks and the GBM, respectively.**

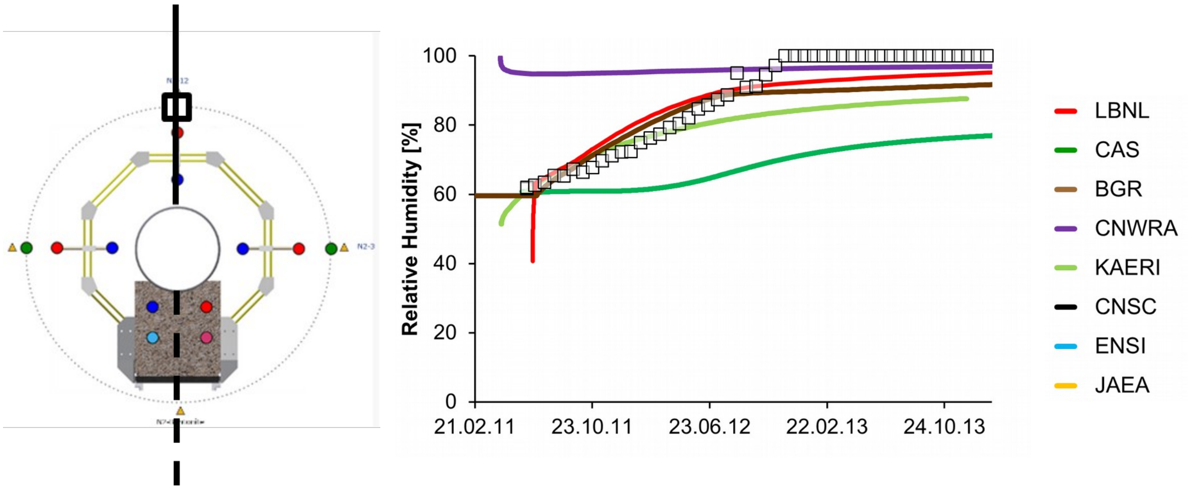

Figure 22: **Measured and modelled relative humidity evolution at 54 cm from the heater surface in the GBM.**

The study focused on the thermal and hydraulic behaviour of the buffer material and clay rock. The mechanical response was less well studied because of the lack of data. Therefore coupled thermal-hydraulic models were also used instead of fully coupled THM modelling (e.g. ENSI team). A poro-elastic model was generally used to describe the mechanical behaviour of both the Opalinus Clay and the buffer materials. This assumption may be sufficient for the Opalinus Clay because the clay rock is still under undisturbed saturated conditions as the maximum temperature is kept under 50 °C in the heating phase (Fig. 24). In the buffer material, complex mechanical deformation may occur. Under high temperature, strong desaturation processes occur, which may lead to local fracturing in the system (BGR/UFZ). High permeability of local channelling, which determines the flow patterns, may be important to consider.

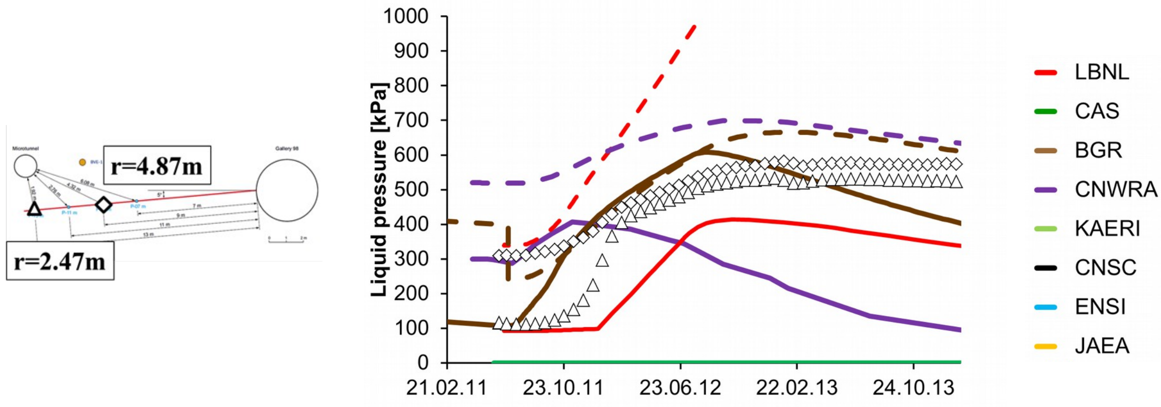

Figure 23: **Measured and modelled pore water pressure evolution at 247 cm (full lines) and 487 cm (dashed lines) from the heater surface in the Opalinus Clay.**

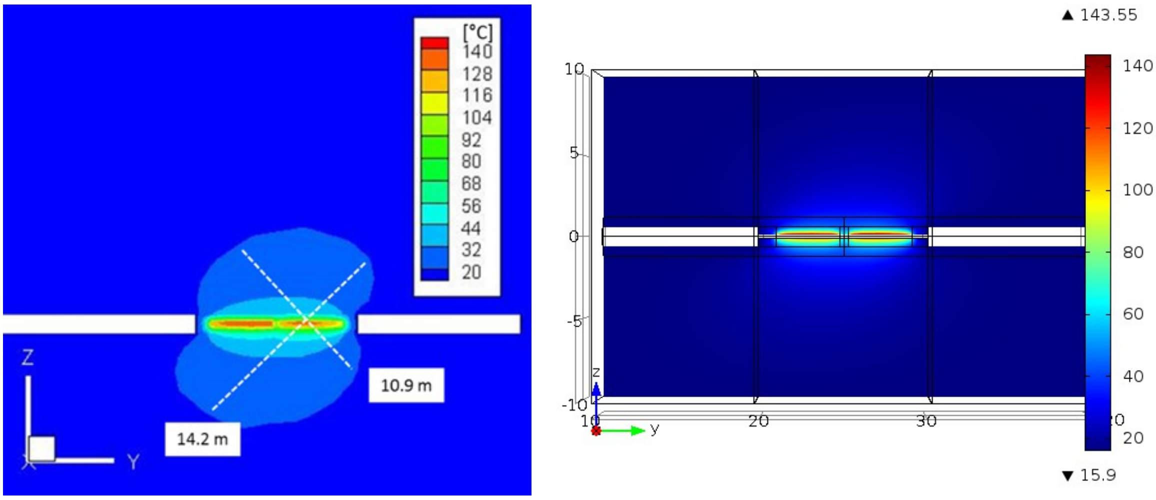

Figure 24: **Temperature distribution calculated by BGR (l) and CNSC (r) taking account of thermal anisotropy.**

5. Discussion and conclusions

To support decision-making for repository site selection and confidence-building for the public, understanding of coupled thermo-hydro-mechanical (THM) processes observed in large-scale demonstration experiments is essential. This requires laboratory and field experiments under in-situ conditions on the one hand, and, on the other hand, powerful numerical tools to interpret the findings from the experiments.
The in-situ HE-E experiment performed in the Mont Terri Rock Laboratory is a valuable example of the understanding of coupled THM processes in Opalinus Clay and buffer material. Extensive experimental data on the evolution of temperature, relative humidity and pore pressure in the buffer materials and surrounding rock allows the teams of the DECOVALEX project to understand the coupled THM processes involved and to validate the developed codes.

In this collaborative research effort, eight research teams have developed mathematical models for interpreting the data gathered in the first 3 years of heating up to a maximum temperature of 140°C. The models applied were mainly based on the theory of heat transport, unsaturated flow and poro-elasticity for continuous porous media to simulate the coupled THM processes. Blind predictions were performed based on the parameters taken from previous studies (HE-D and column tests) and interpretative modelling carried out to improve the understanding of the THM responses of the buffer materials and clay host rock.

Anisotropic properties of the Opalinus Clay and strong coupling between the thermal and hydraulic properties of the buffer materials (granulated bentonite mixture, bentonite blocks and sand/bentonite mixture) were considered. The models were able to reproduce the main physical processes observed in the experiment.

The heater surface temperature is well reproduced by applying the power input as a boundary condition, which indicates that the thermal conductivity of buffer and host rock are correct.

The temperature evolution in the buffer and general trends of the relative humidity evolution are relatively well reproduced. However, agreement between measured and modelled temperature and relative humidity in the middle of the buffer was not as satisfactory as at other locations. This problem could not be addressed by any of the different sensitivity analyses performed by the teams to explore the different processes. This might indicate that the different models have overlooked a process (e.g. structural change of bentonite pellets from triple to dual porosity).

Generally, the temperature field can be well reproduced, which is mainly controlled by thermal conductivity in the heat conduction process. The thermal conductivity of unsaturated materials is well characterised in the laboratory and depends strongly on the water saturation. The distribution of water saturation (relative humidity) is again determined by unsaturated or multiphase flow models taking vapour diffusion into consideration. Due to different approaches applied for interpreting the relationship between relative permeability and water saturation as well as retention function, a wide range for the time required for resaturation of buffer materials was calculated. This uncertainty cannot unfortunately be eliminated by sensitivity analysis of parameters used in the individual models. However, the models may be improved if more laboratory data on the hydraulic properties of unsaturated buffer material are available.

A thermally induced pore water pressure increase in the rock mass can be interpreted reasonably well by applying the thermal expansion coefficient for water in the elastic model coupled with consolidation processes. A swelling/shrinkage model introduced by some teams may only affect the mechanical behaviour, because a change in hydraulic properties (porosity and permeability) was generally not considered in the current state.

The trend of pore water pressure evolution was predicted on the basis of an upscaling exercise (from the small scale HE-D test to the 1:2 scale HE-E experiment) without consideration of the hydraulic properties in the EDZ because almost no EDZ was detected in the HE-D borehole (30 cm in diameter) and a very limited EDZ around the HE-E micro-tunnel (130 cm in diameter) was found. In the further upscaling exercises to the real scale, the EDZ will probably have to be taken into account.

All the important measurement trends associated with ongoing THM processes were reasonably well reproduced qualitatively and quantitatively in most cases. The analysis of the results from the prediction and interpretation confirms that the main processes in the system have been understood and captured using the developed models and associated parameters with respect to the thermal and hydraulic aspects:

- Saturation of the buffer
- Dependence of thermal conductivity on saturation
- Supply of water from the rock mass (characterisation of the saturation state and pore pressure in the rock around the tunnel).

Nevertheless, the short-term analysis does not necessarily ensure that all the key processes have been identified and implemented in the models and/or correctly calibrated for longer-term simulations. Some processes might not be perceived in short-term observations and current model simulations, but may gain in importance for long-term predictions:

- Changes in the pore structure in the buffer material (from triple porosity material to single porosity material) could significantly affect the transport properties of the buffer material and hence significantly change the estimated resaturation time
- Sophisticated mechanical models for the buffer material were not emphasised in the calibrations, in general, and may deserve more attention, especially under high temperature
- Processes such as thermal or chemical osmosis were not considered
- In the long run, water fluxes in the buffer are likely to decrease (from their already very small magnitude). This means that the validity threshold of Darcy's flow used as the main water flux driver might be exceeded. This could also significantly affect the estimation of resaturation time.

The results obtained in this context are valid only for these particular conditions. The dimensions of real disposal galleries are different to the diameter of the HE-E micro-tunnel and this will lead to longer re-saturation times, which may require further model upscaling. The back pore pressure of the rock in the HE-E surroundings is fairly low (even in the Mont Terri Rock Laboratory). A higher back pressure might significantly accelerate the re-saturation process.

However, according to the current status of knowledge, these potential discrepancies are not believed to significantly affect the safety function. Upcoming results from the column tests and the HE-E experiment with the focus on dismantling and ‘post-mortem’ analysis will further improve the understanding of ongoing processes. The additional experimental results will be compared with the "predicted" results of the models presented here. This will help to increase confidence in the THM models and in process understanding.

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