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EVALUATION AND IMPROVEMENT OF THE THM MODELLING CAPABILITIES FOR ROCK SALT REPOSITORIES

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Abstract. *This paper provides a summary description of the selected results obtained in the frame of the THERESA- project cosponsored by the European Commission (EC). The numerical modeling of coupled thermal-hydraulic-mechanical (THM) processes with impact on repository long-term safety was focused on simulation of a number of representative laboratory experiments on rock salt samples. The scope of these calculations was the validation of the actual capabilities of the constitutive model and to identify needs for further improvements of the model. The measured development of volumetric strains and permeability in the samples during loading process was compared posterior to calculation results.*

1 INTRODUCTION

The objectives of the European Community project THERESA ("Coupled thermal-hydrological-mechanical-chemical (THMC) processes for application in repository safety assessment") [1] are to develop, verify and improve the modelling capabilities and capacities of mathematical models and computer codes for coupled processes for use in performance assessment of the long-term safety of nuclear waste repositories in crystalline rocks and rock salt. The Work Package 3 (WP3) of this project focused on the evaluation and improvement of numerical modelling capabilities for assessing the performance and safety of nuclear waste repositories in rock salt, with particular regard to the long-term evolution of the excavation damaged zone (EDZ), considering thermal-hydraulic-mechanical processes.

Furthermore in this Work Package triaxial compressive test on rock salt samples and a large-scale test on a hollow salt cylinder were performed and then considered for an unconventional benchmark analysis. The evolution of the THM processes occurring during these tests was calculated using the finite element code ADINA [2]. A new viscoplastic constitutive model for rock salt that can describe the volumetric strain (dilatancy) and the damage of the rock has been proposed and implemented in this code. The rock damage (i.e. micro cracks or fractures) was judged by criteria for shear and tensile fracture and by the dilation criterion. The main attention focused on the simulation of strains and permeability development the rock salt samples. Subsequently, the calculated strain rates were compared toexperimental data.

2 CONSTITUTIVE MODEL FOR ROCK SALT

The constitutive model proposed in this project is based on the assumption of small strains, where the total strain rate, $\dot{\varepsilon}_{tot}$ is split into elastic and viscoplatic parts as follows:

$$\dot{\varepsilon}_{tot} = \dot{\varepsilon}_{el} + \dot{\varepsilon}_{vp} \tag{1}$$

$\dot{\varepsilon}_{el}$ elastic strain rate tensor

$\dot{\varepsilon}_{vp}$ viscoplastic strain rate tensor

The elastic behaviour is assumed to be time-independent. Furthermore, the viscoplastic strain rate tensor is decomposed into a viscoplastic strain rate tensor by constant volume and a viscoplastic strain rate tensor due to damage that considers the volume change, such as dilatancy or compaction of the material:

$$\dot{\varepsilon}_{vp} = \dot{\varepsilon}_{vp}^{c} + \dot{\varepsilon}_{vp}^{d} \tag{2}$$

$\dot{\varepsilon}_{vp}^{c}$ viscoplastic strain rate without volume change

$\dot{\varepsilon}_{vp}^{d}$ viscoplastic strain rate due to damage which describes a volumetric strain

For each viscoplastic strain rate, an associated flow rule is used:

$$\dot{\varepsilon}_{vp} = \gamma < \Phi\ (F(\sigma)) > \partial F / \partial \sigma \tag{3}$$

where

$\gamma = a_1 \exp(-a_2 / T)$ is the fluidity parameter,

a_1 and a_2 are material constants and T is temperature;

The term $\Phi\ (F)$ denotes a monotonic function of the yield function (F). The meaning of the brackets < > is as follows:

$$< \Phi\ (F) > \ = \ 0 \qquad \text{if } F \leq 0 \tag{4}$$
$$< \Phi\ (F) > \ = \ \Phi\ (F) \qquad \text{if } F > 0$$

The function $\Phi\ (F)$ is defined as:

$$\Phi\ (F) = (F - F_o)^{\mathrm{m}} \tag{5}$$

where m is an arbitrary constant and F_o is the uniaxial yield stress and set to zero for instance. For our viscoplastic model, the functions F^c and F^d are defined as follows:

$$F^c = q^2 \quad \text{(without volume change)} \tag{6}$$

$$F^d = n_1\, p^2 + n_2\, q^2 \tag{7}$$

where

p is the mean stress and q is the standard stress deviator,

n_1, n_2 are material functions of the volumetric strain, ε_{vol} ,

and expressed as:

$$n_1 = c_1\, (q^2/p^2 - c_2\, (\eta_0 + \varepsilon_{vol}\,)/(1 + \varepsilon_{vol})) \tag{8}$$

$$n_2 = 1 - c_3 .\ n_1\, p^2 / q^2 \tag{9}$$

with c_1, c_2, and c_3 being material constants to be evaluated by laboratory tests. In the present approach η_0 is the initial porosity of the undamaged rock salt.

This viscoplastic material model for damage is based on the mathematical formulation proposed by Hein [3] for granular materials, such as crushed salt, and was implemented in the finite-element code ADINA [4]. Separate criteria for shear and tensile fracture and a compression-dilation boundary [5, 6] are available to judge the damage of rock salt (i.e. micro-cracks or fractures):

- Shear stress criterion for compression

$$\tau_f \geq b \ |\sigma_m|^p \tag{10}$$

where

τ_f : predicted shear stress at failure

σ_{m} : mean stress

b and *p* are fitting parameters.

- **Tension-induced failure** is assume if the max. principal stress exceeds a tension of 1MPa.

- Compression-dilation boundary

$$\tau_{cd} \ \geq \ f_1 \sigma - f_2 \ \sigma_m^{\ 2} \tag{11}$$

where f_1 and f_2 are fitting parameters.

The permeability of the damage rock salt is correlated to the dilatant volumetric strain according to the following preliminary function reported in the literature [7]:

$$k \ = A \cdot \varepsilon_{vol}^{\ \ B} \tag{12}$$

where

k: permeability of rock salt;

A and *B* are material parameters given by different authors and types of the rock salt.

Recently, a new permeability model for rock salt has been proposed by [8] and is presented below together with the material parameters. This model represents a relation between the mean stress and rock porosity:

$$k = \frac{k_{tp}}{\left(\frac{\phi}{\phi_{tp}}\right)^{-p_1} + \left(\frac{\phi}{\phi_{tp}}\right)^{-p_2}} \tag{13}$$

with

$$k_{tp} = a_k \cdot exp\left(-\ p_c \cdot b_k\right)$$
$$\phi_{tp} = a_\phi \cdot exp\left(-\ p_c \cdot b_\phi\right)$$

3 MODEL CALIBRATION

In order to adjust the material parameters and to demonstrate the applicability of the material model to describe the dilatant volumetric strain of rock salt, a number of different triaxial laboratory tests were investigated numerically. The calculated strain rates were compared to experimental data. The influence of different material parameters on the numerical results was studied and described in Reference [9]. In the framework of the

THERESA project some new numerical analyses of various laboratory transient-creep experiments [10] have been performed. A test conducted on rock salt from the Asse mine for which the volumetric strain rate was measured has been numerically analysed. The cylindrical specimen had a diameter of 86.5 mm, a length of 175.0 mm, and a density of 2160 kg/m3 at the beginning of the test and was subjected to an axial compression with controlled strain rates of 10^{-7} 1/s and a horizontal confining pressure of 1MPa. In this analysis it was assumed that the dilation of the samples starts immediately after loading (i. e. the short time elastic compaction of the sample was not modelled). A comparison of the measured and calculated strain-stress curves, as well as the development of volumetric strains, are presented in the Figures 1 and 2, respectively.

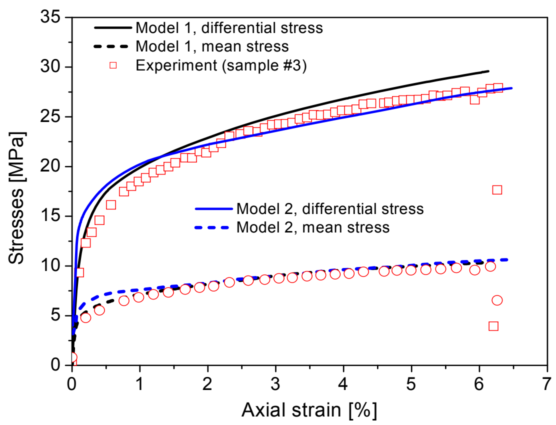

Figure 1: Development of stresses as a function of axial strain; Model 1, with damage parameters fitted on strength tests (strain rate of 1E-05 1/s), Model 2, new parameters set.

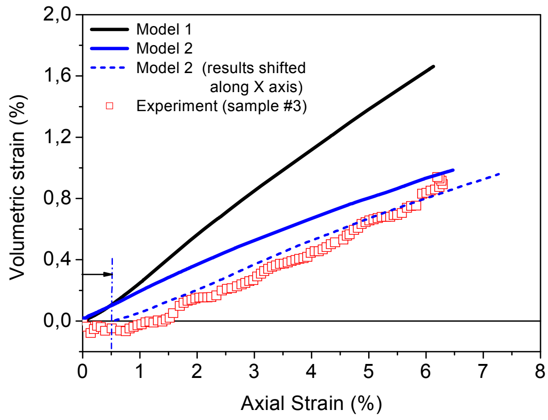

Figure 2: Comparison of measured and calculated volumetric strains for two sets of parameters.

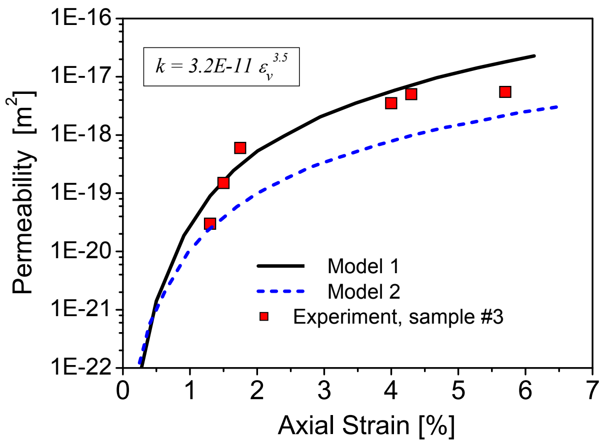

Figure 3: Permeability of the sample during the transient creep test and the calculated evolution of the permeability for two sets of parameters of the calculation results along the horizontal axis lead to a good overall correlation to measurements (Model 2, dashed curve).

Using the calibrated parameters on earlier laboratory transient creep tests the model predicts the development of effective and mean stresses quite well, but the volumetric creep strain over-estimates the actual measurements (Model 1). With a minor adjustment of the damage parameters it can be recognised that the results obtained are in better agreement to the experimental data (Model 2).

The porosity-permeability relation described by the equation (12) was used to calculate the development of permeability of the sample. Figure 3 shows the permeability of rock salt calculated from the obtained volumetric strain in comparison with the laboratory measurements. In Tab. 1 are the parameters obtained from the model calibration summarized.

Table 1: Material parameters for rock salt

Properties	**Parameters**
Thermo-elastic properties	E = 27 GPa; ν = 0.25; α = 4.2E-05 1/*K*
Transient creep	a_0 = 0.018; a_1 = 240; a_2 = 0.112; Qc /RT = 6495
Viscoplastic damage	m = 2.25; c_1 = 0.3; c_2 = 400; c_3 = 2; η_0 = 0.02%
Hydraulic properties Equations (12) and (13)	A = 3.2E-11; B =3.5
	p_1 = 4; p_2 = 1; a_k = 4.27E-14; b_k = 1.26; a_Φ = 0.0263; b_Φ = 0.3093

4 LABORATORY TEST CASE

In order to demonstrate the capabilities and suitability of the calibrated models to calculate EDZ evolution and reconsolidation of the damaged salt, a laboratory benchmark test was designed and conducted [10]. A schematic representation of the triaxial test cell is shown in Figure 4. The test was performed in two steps (test case TC2A and TC2B, respectively). After two load steps at 11 MPA and 19 MPa deviatoric stress of the sample without permeability increase, the sample was removed from the apparatus and inspected. Afterwards, the sample was installed again and the experiment was restarted with several loading steps, a reconsolidation phase and a phase of elevated temperature. The evolution of the stresses during the second phase (TC2B) is presented in Figure 5. More details are given in the THERESA laboratory test report [10].

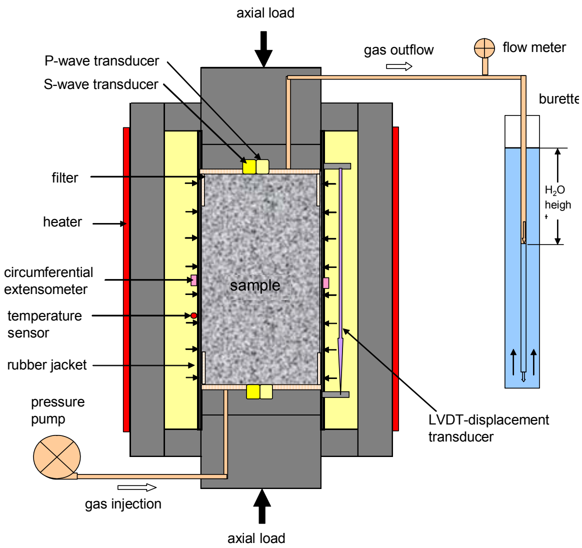

Figure 4: Schematic assembly of a salt sample in the triaxial cell [10].

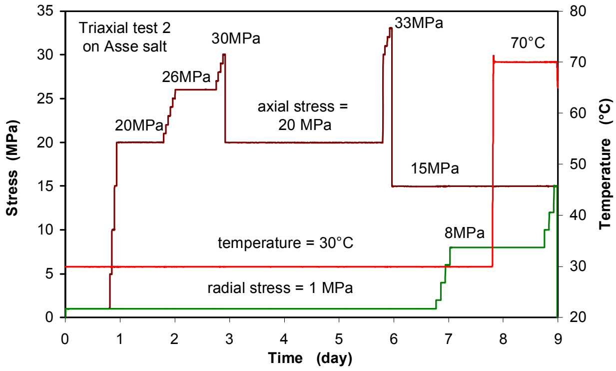

Figure 5: Load conditions applied to the benchmark sample in phase TC2B [10].

5 NUMERICAL SIMULATION

A triaxial compressive test (TC2B) conducted on Asse rock salt was proposed for the benchmark analyzes. The evolution of the THM processes occurring during those tests was simulated using the ADINA code. The attention was focused on the simulation of strains and permeability development in the rock salt samples. Subsequently, the calculated strain rates were compared to experimental data. The main objectives of the benchmark calculations are the validation of the actual capabilities of the constitutive model and to identify needs for further improvements of the model.

5.1 Description of the model and boundary conditions

The model geometry used for the analysis is the same as that of the experimental cylindrical rock salt sample with a diameter of 100 mm and a height of 190 mm. The initial and boundary conditions are assumed as follows:

- Thermal: The whole sample was kept at room temperature of 30°C for about 8 days after this period the temperature was rapidly increased to 70°C and kept constant until the test ends.
- Hydraulic: Boundaries are impervious except for the both top boundaries to permit gas in- and outflow, where gas pressure at the bottom of 0.5 MPa and the atmosphere pressure at top were imposed.

- Mechanical: At the top boundary a time dependent vertical stress and at the outer cylinder surface a radial stress was applied. The bottom surface of the model was fixed in the normal and horizontal directions.

Details of the loadings are given in Figure 5 and the laboratory tests report [10]. The parameters adopted in the simulation coincide with those assumed in the previous model calibration and are summarized in Tab. 1.

5.2 Calculation results and discussions

The comparison of the calculated strains with the strains measured is shown in Figure 6 on which the symbols are the experimental data and the continuous lines are the response of the model. There are same differences during the second creeping stage due to the fast increase of the vertical stress from one to 20 MPa. During the next moderate increase and decrease of the loading stages there is a better agreement between the experimental and predicted strains. In our case the calculated salt permeability using both available relations shows differences in the first loading stages (Figure 7) because of the assumed initial porosity of the salt sample as near zero (η_0=0.0002). Taking into account that the initial porosity of the sample was about 0.2% and the corresponding permeability of about 10^{-19} m^2, a new simulation will match quite well with the measured behaviour. The increasing temperature and also the confining pressure have different influences on the actual results. Unfortunately, it must be mentioned that at the moment there are too few experimental results available to be sure that our assumptions are correct.

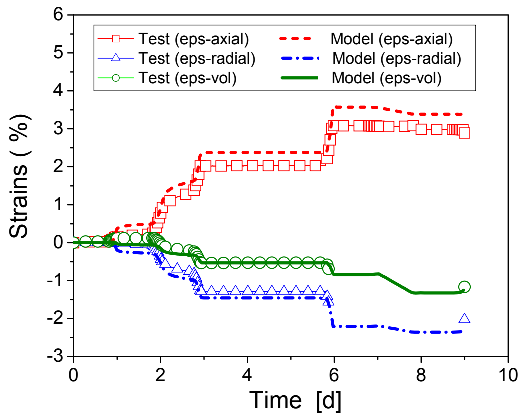

Figure 6: Comparison of measured and predicted axial, radial and volumetric strains.

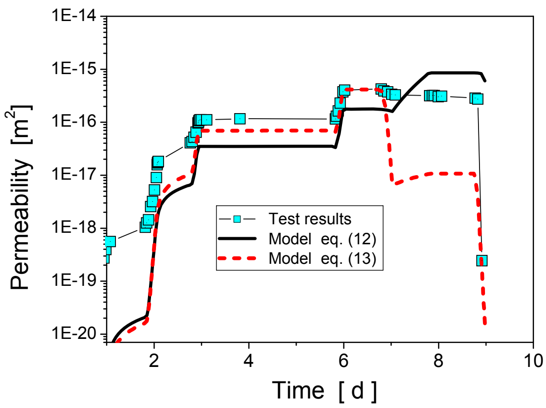

Figure 7: Permeability of the sample during the transient creep test TC2B and the calculated evolution of the permeability with two different relations.

The distributions of void volume fraction and strains in the model at the time t = 8.3 days are shown in Figure 8. Due to the experimental boundary condition at the upper and lower surfaces of the sample, large strain gradients and the failure of rock salt were calculated. This is not surprising as the case under study is characterized by small dimensions and a rapid change in stress loading and unloading. The effect will also influence the hydraulic behaviour of the sample material at these locations. It must be pointed out that the numerical model used is a simplified hydro-mechanical formulation based on Darcy' law and a saturated porous media which are questionable with regard to gas flow through a viscous rock at high temperature.

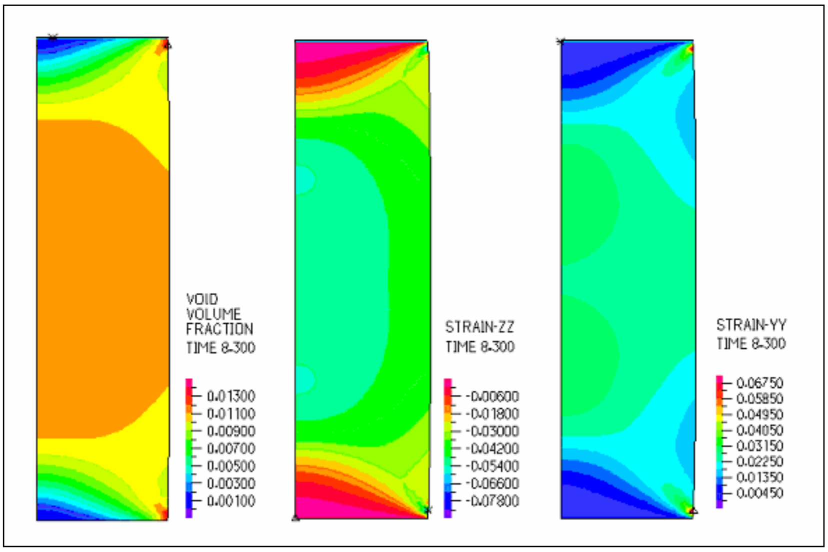

Figure 8: The spatial distributions of the void volume fraction, axial and horizontal strains after 8.3 days.

12 CONCLUSIONS

The numerical simulation results of the laboratory benchmark tests, performed on rock salt have shown a quite good agreement with experimental data. The mathematical formulation of the constitutive model is simple and can be easily implemented in different numerical codes. The model is suitable to describe the main hydro-mechanical behaviour of the rock salt such as transient creep, volumetric strain and material damage. In the case of the sealing (re-consolidation) of the damaged salt, there is still a considerable difference between the model and experimental data. A future improvement of the proposed model is required.

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