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Development of Material Models, Implementation in Finite-element Codes, and Validation

A. Pudewills

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Alexandra Pudewills

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Numerische Modellierung der Langzeitentwicklung von Auflockerungszonen

Entwicklung von Stoffmodellen, Einbau in Finite Elemente Rechenprogramme und Bewertung

Zusammenfassung

Die Konstruktion von tiefen, untertägigen Hohlräumen beeinflusst den ursprünglichen Spannungszustand des umliegenden Gebirges. Dieser Effekt kann unter Umständen zu Mikrorissen und Änderungen der hydraulischen Eigenschaften des Gesteins im Nahfeld von Hohlräumen führen. Für die Langzeitsicherheit von Endlagern in Steinsalzformationen spielt die Entwicklung von solchen Auflockerungszonen (EDZ) und deren hydro-mechanische Eigenschaften eine wichtige Rolle aufgrund ihrer Bedeutung beim Nachweis der Integrität der geologischen und geotechnischen Barrieren in einem Endlager.

Im Rahmen des EU-Projektes NF-PRO, Arbeitspaket WP4.4, werden Rechenmodelle zur Simulation der Bildung und Weiterentwicklung von Auflockerungen in der Umgebung einer Endlagerstrecke entwickelt. Für diese Untersuchung wurden die vorhandenen Finte-Elemente Programme mit zeit- und temperaturabhängigen Stoffmodellen verbessert. Ein neues viskoplastisches Materialmodell zur Beschreibung der Dilatanz und Schädigung von Steinsalz wurde implementiert und die Materialparameter wurden an Laborversuche angepasst. Weiterhin wurde die Langzeitentwicklung der Auflockerungszone in der Umgebung eines Tunnels auf der 700 m-Sohle eines Salzbergwerks modelliert. Der Vergleich der Rechenergebnisse und der in situ Messungen wird dargestellt. Die Übereinstimmung zwischen den berechneten Konvergenzraten, der Spannungsentwicklung sowie die Änderung der Salzpermeabilität in der Auflockerungszone und die gemessenen Werte deutet auf die Richtigkeit des verwendeten Rechenmodells.

Development of material models, implementation in finite-element codes, and validation

Abstract

Construction of deep underground structures disturbs the initial stress field in the surrounding rock. This effect can generate microcracks and alter the hydromechanical properties of the rock salt around the excavations. For the long-term performance of an underground repository in rock salt, the evolution of the "Excavation Disturbed Zone" (EDZ) and the hydromechanical behaviour of this zone represent important issues with respect to the integrity of the geological and technical barriers. Within the framework of the NF-PRO project, WP 4.4, attention focuses on the mathematical modelling of the development and evolution of the EDZ in the rock near a disposal drift due to its relevance on the integrity of the geological and technical barriers.

To perform this task, finite-element codes containing a set of time- and temperature-dependent constitutive models have been improved. A new viscoplastic constitutive model for rock salt that can describe the damage of the rock has been implemented in the finite-element codes available. The model parameters were evaluated based on experimental results. Additionally, the long-term evolution of the EDZ around a gallery in a salt mine at about 700 m below the surface was analysed and the numerical results were compared with in-situ measurements. The calculated room closure, stress distribution and the increase of rock permeability in the EDZ were compared with in situ data, thus providing confidence in the model used.

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1 Introduction

The excavation of underground repositories leads to the perturbation of the initial lithostatic stress state in the rock mass around the openings, creating microcracks and degrading the hydromechanical properties. Over time, due to creep-strain rates of the rock salt and the increased support of the compacting backfill, the extension of the **E**xcavation **D**isturbed **Z**one (EDZ) will be reduced. For the long-term performance of a geological repository, the evolution of this zone represents an important issue with respect to the integrity of the geological and technical barriers.

The aim of numerical modelling is to predict the development and evolution of the EDZ under different conditions and its interaction with the backfill material. To investigate the processes in the EDZ, numerical models with adequate constitutive laws are under development. In this work package, attention focuses on the modelling of hydromechanical processes in the near field of a disposal drift in salt and clay formations.

In the reporting time, a new material model for rock salt that can describe the damage of the rock has been implemented in the finite-element codes MAUS [1] and ADINA [2]. According to this model, the total strain rate is given as the sum of elastic and viscoplastic strain rates. The viscoplastic strain rate is decomposed into a part without volume changes of the material and a second one taking into account the volume changes due to the damage. In this case, the viscoplastic flow function depends on mean stress, deviatoric stress, and volumetric strain.

First, some relatively simple analyses of various laboratory transient-creep experiments were performed. In these tests the volumetric strain (dilatancy) of the samples was measured. The calculations included the calibration of the model parameters and also a first validation of the model by a comparison of numerical results with experimental data from an independent test (i.e. not used for finding the constants). The influence of different material parameters on the calculation results was also studied.

In a next step, the model's capability of simulating the development of EDZ near a gallery in rock salt was studied. The problem under consideration as that of a 37 years old gallery with a diameter of 3 m and located at a depth of 700 m from the surface in the Sondershausen salt mine [3]. The numerical results were compared with in situ measured closure rates, stresses, and rock salt permeability. Based on the experience gained from the evaluation of laboratory tests and in situ measurements, a predictive calculation of an emplacement drift in a conceptual repository will start in the next phase of the NF-PRO project.

The report will be organised as follows. The next section will present the constitutive model of rock salt and its extension to describe the rock damage. Validation of the damage model by laboratory tests and parameter studies will be described in section 3. Numerical analysis of the development and evolution of EDZ in the near field of a 37 years old excavation, shall be given in section 4 and, finally, some concluding remarks will be presented in section 5.

2 Constitutive model for rock salt

The constitutive model proposed 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:

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

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

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

For each viscoplastic strain rate, an associated flow rule is used (i.e. the viscoplastic potential function is the same as the yield function and the viscoplastic strain increment vector will be associated with the yield surface [4])

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

where

$\gamma = \mathrm{a}_1 \exp(-\mathrm{a}_2 / \mathrm{T})$ is the fluidity parameter;

a_1 and a_2 are material constants, T is temperature;

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

$$\begin{aligned} < \Phi\,(F) > &= 0 \qquad \text{if } F \le 0 \\ < \Phi\,(F) > &= \Phi\,(F) \qquad \text{if } F > 0 \end{aligned} \tag{4}$$

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

$$\Phi\,(F) = (F - Fo)^{m} \tag{5}$$

in which *m* is an arbitrary constant and Fo is the uniaxial yield stress and set to zero for instance. For our viscoplastic model, the functions F^{c} and F^{d} are as follows:

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

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

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:

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

$$n_2 = 1 - c_3 . n_1 p^2/ q^2 \quad (9)$$

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 undisturbed rock salt .

The viscoplastic material model for damage proposed is based on the mathematical formulation proposed by Hein [5] for granular materials, such as crushed salt, and was implemented in the finite-element codes ADINA and MAUS. A detailed description of the finite-element algorithm is given in [5, 6]. This algorithm was also used to implement the current damage model in both programs.

Furthermore, separate criteria are available for shear and tensile fracture [7] and a compression-dilation criterion [8] to judge the damage of rock salt (i.e. microcracks or fractures):

- Shear stress criterion for compression

$$\tau_f \geq b\, |\sigma_m|^{p} \quad (10)$$

where

τ_f : predicted shear stress at failure
σ_m : mean stress
b and p are fitting parameters.

A safety factor is defined as:

$$FS = \tau_{oct} / \tau_f \quad (11)$$

with τ_{oct} being the actual octahedral shear stress. Under compression loads, failure will occur if $FS > 1$.

- Tension-induced failure is assumed if the maximum principal stress exceeds a tension limit of 1 MPa.

- Compression-dilation boundary:

$$\tau_{oct} \geq f_1\sigma - f_2\,\sigma_m^{2} \quad (12)$$

where f_1 and f_2 are fitting parameters.

Two preliminary relations between permeability and the volumetric strain given in references [9] and [10] are used to calculate the permeability of the rock salt:

$$k = A \cdot \varepsilon_{vol}^{B} \quad (13)$$

k : permeability of rock salt and A and B are material parameters.

3 Validation of the proposed damage model

In order to verify the implemented material model and to demonstrate the applicability of the model to describing 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 as well. Taking into account the preliminary relation given in equation (13), the permeability of the samples was computed.

3.1 Simulation of transient creep tests

A transient creep test conducted on WIPP rock salt sample [10] for which the volumetric creep strain rates are available was selected for the numerical analyses. The cylindrical sample was subjected to an axial compression of 28 MPa and a lateral confining pressure of 3 MPa. The tertiary creep test lasted 1.2 hours. For the calculation, a simple one-axial symmetric element was considered. The material parameters used for simulation are summarised in Table 1. The shear stress, tensile stress, and the compression-dilation criterion were not used in this analysis. The dilation of the samples was assumed to start immediately after loading.

Tab. 1: Material constants used in the numerical analysis

Thermoelastic properties	E = 36 GPa; ν = 0.27; α = 4.2E-05 1/*K*
Viscoplasticity, equations (3), (5)	a_1 = 2.08E-05 1/s; a_2 = 6520; *m* = 2; T = 293 *K*
Dilatancy, equations (8), (9)	c_1 = 0.7, c_2 = 500, c_3 =1
Permeability, equation (13)	A = 3.2 E-11; B = 3.5 ref. [9] and A = 2.13 E-09; B = 3 ref. [10]

Figure 1 shows the calculated development of axial, radial, and volumetric strains compared with the experimental data given in ref. [10]. As evident from this figure, the calculation predicts the dilatant volumetric creep strain of the sample quite well. Figure 2 shows the resulting permeability of the sample as a function of volumetric strain for both sets of parameters. The calculated values are in the ranges of in-situ permeabilities of rock salt measured in the near field of a large excavation in the Asse mine [9]. For illustration, the measured permeabilities are also depicted in this figure.

The second problem considered was that of a similar triaxial creep test. For this test, the numerical results obtained using the Hou/Lux damage model [11] over a period of 12 days are presented in [12]. Fig. 3 shows the numerical results obtained with the proposed model in comparison with the results from the Hou/Lux constitutive model. Unfortunately, the volumetric strain is not available, but it can be calculated easily from axial and radial strains. In this case, a new set of material constants c_1 and c_2 was fitted to the results available. A good overall correlation was achieved. For this example, a sensitivity study was made to determine the influence of both damage parameters c_1 and c_2 on the calculated volumetric strains (Fig. 4).

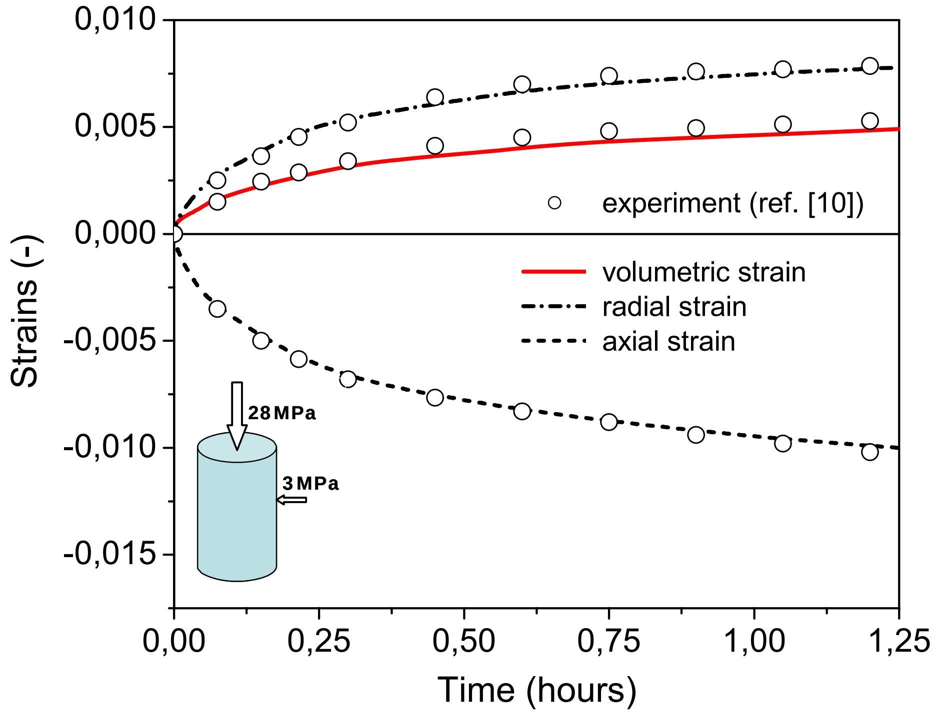

Fig. 1: Comparison between measured creep strains and calculation results

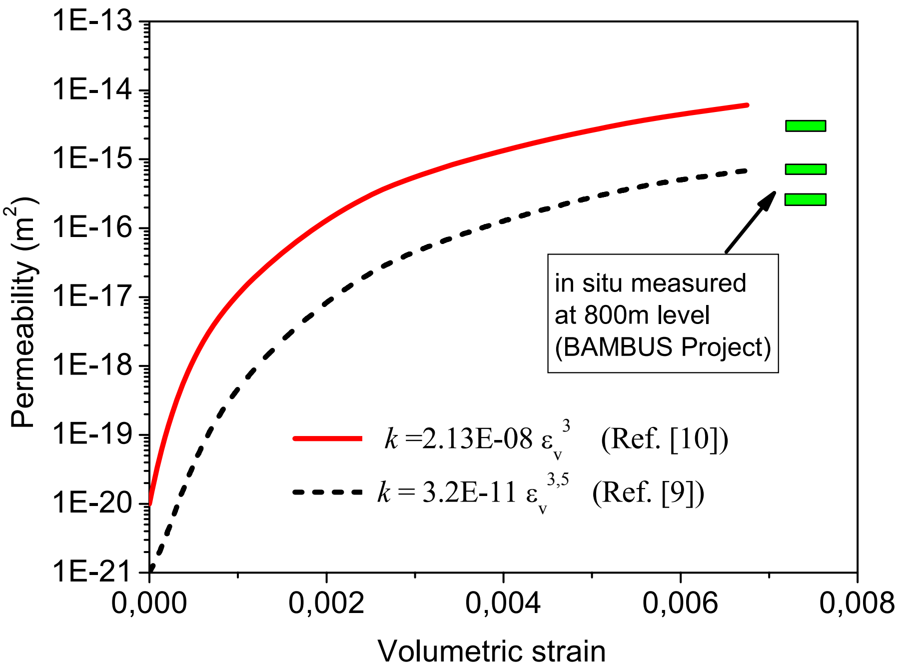

Fig. 2: Permeability of the sample during a transient creep test, calculated using two different relations. For illustration, the permeabilities measured around a large gallery in the Asse mine [9] are plotted.

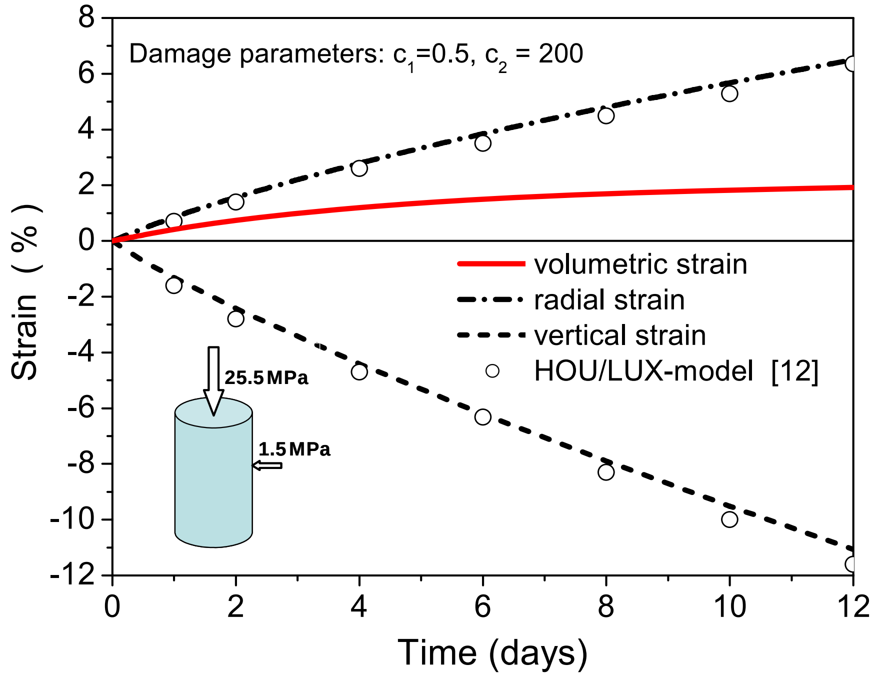

Fig 3: Comparison between results calculated with the proposed damage model and the Hou/Lux model [12]

This parameter study indicates that the constant c_1 influences the shape of the calculated curves, but not the final value of the volumetric strain if the assumed boundary conditions and the creep parameters of the rock remain the same. The parameter c_2 directly limits the maximal amount of the calculated dilatancy. As can be seen from Fig. 4, the increase of c_2 from a value of 200 to 300 induces a relevant reduction of the volumetric strain maximum.

In Fig. 5 the calculated evolution of the permeability in the specimen is presented for two sets of parameters. As expected, the calculated permeabilities at the end of the numerical experiment are identical.

3.2 Simulation of short-time triaxial compression tests

The short-time compression tests (or strength tests) are widely used in the laboratory to determine the effect of confining pressure on the failure behaviour of rocks. The cylindrical specimen is subjected to an axial compression with controlled strain rates and a horizontal confining pressure. Depending on the loading velocity (i.e. strain rates) and the lateral pressure applied, a volumetric deformation of the sample will appear.

In this section two such tests performed by BGR and TU-Clausthal [13] shall be analysed. A comparison of the measured and calculated strain-stress curves as well as the development of volumetric strains are presented in Figures 6 and 7. The main attention in this analysis focused on the simulation of volumetric strains. The failure of the specimens has not yet been modelled.

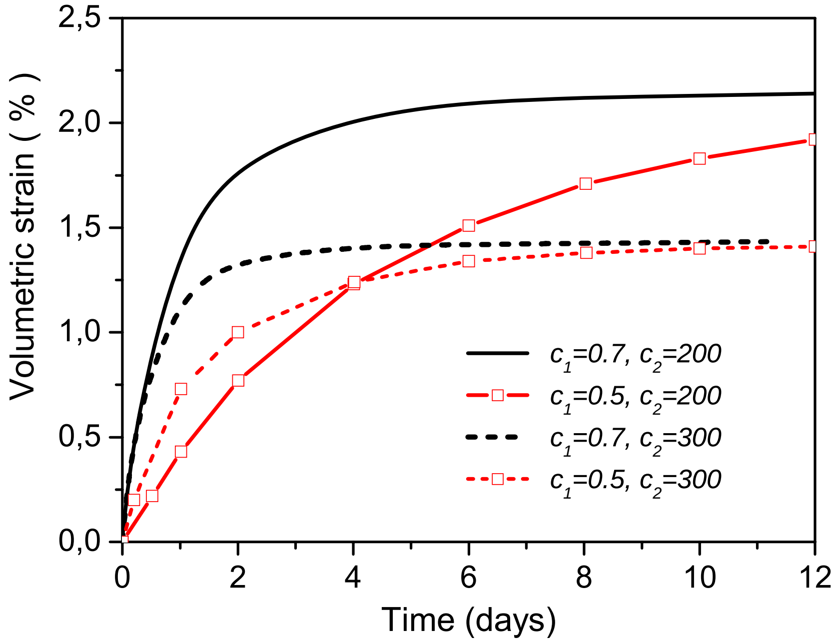

Fig. 4: Development of volumetric strain for various values of model parameters

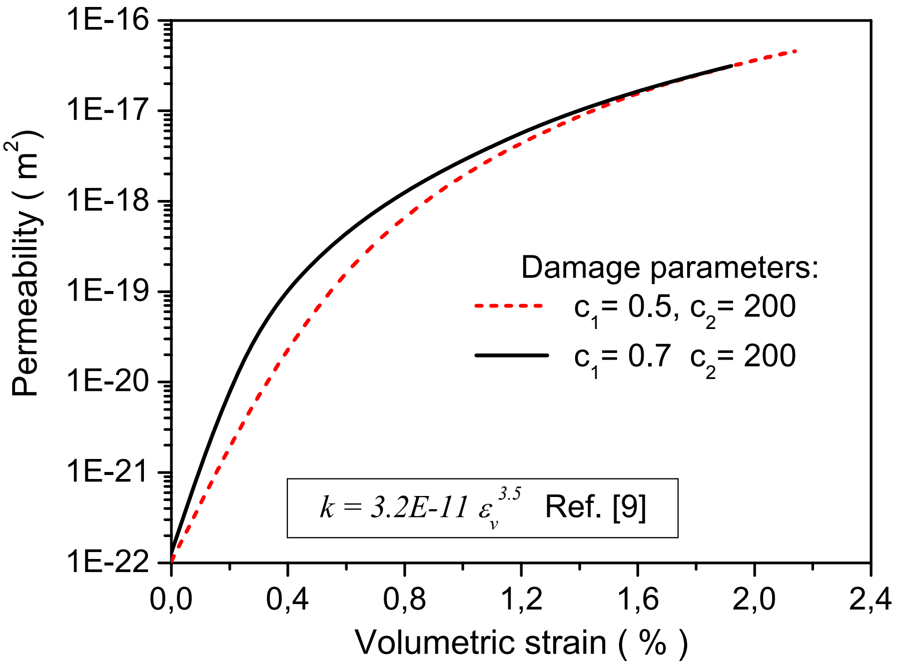

Fig. 5: Permeability as a function of volumetric strain for two sets of parameters

It should be noted that these tests are not representative of in-situ strain-stress conditions because of the very fast loading velocity (i.e. axial strain rates of 1E-5 to 1E-6 1/s) which are two to three orders of magnitude higher than expected around an opening in the underground. Nevertheless, the laboratory tests allow to verify the material model developed.

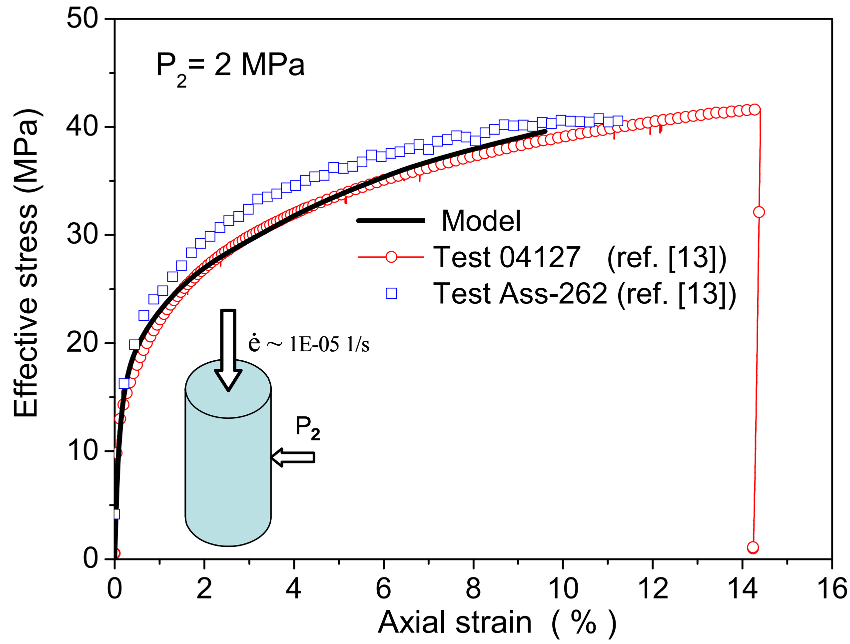

Fig. 6: Comparison of experimental stress-strain curves and calculation

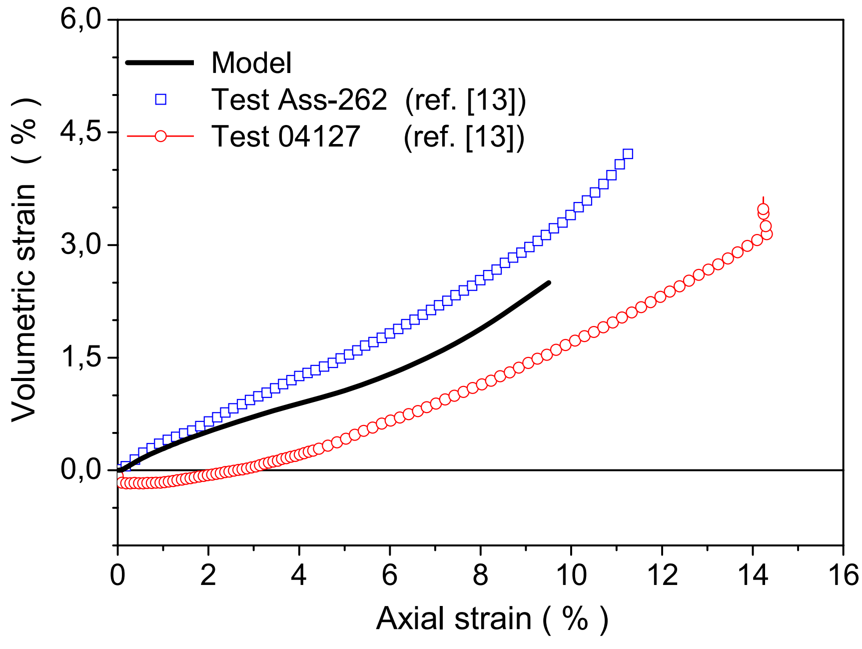

Fig. 7: Development of volumetric strains as a function of axial strain and comparison with calculation results

4 Modelling of the EDZ around a gallery in rock salt

To illustrate the capability of the material model and the codes used, the long-term evolution of the EDZ around a 37 years old gallery in a rock salt formation was analyzed. The circular gallery, EU-1, with a radius of 1.5 m is located 700 m below the surface in the Sondershausen salt mine. The room closure rates, the radial stress, and permeability distribution after 37 years were measured in situ and are given in references [3] and [14].

To perform the numerical analyses with a reasonable numerical effort, a 2D model of a quarter geometry was used, assuming plane strain conditions. Fig. 8 shows the finite-element model and the assumed boundary conditions.

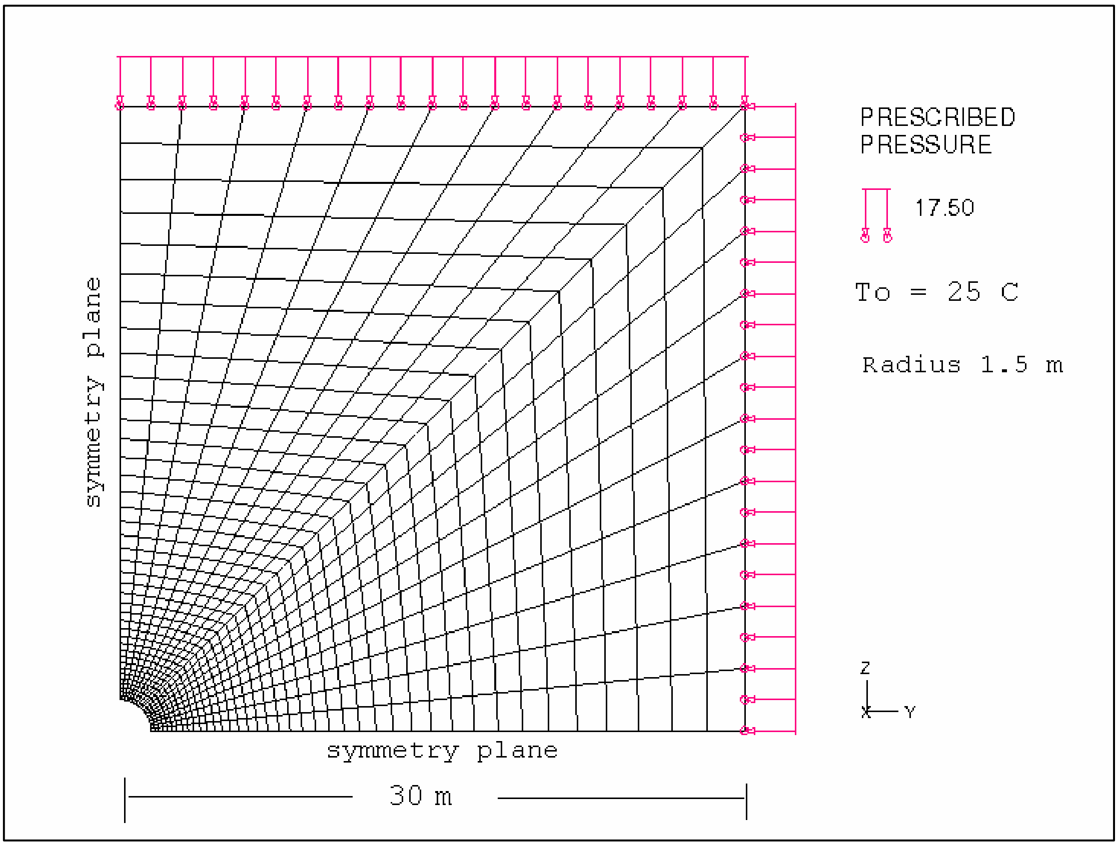

Fig. 8: Finite-element mesh and initial boundary conditions

The radial convergences of the gallery calculated for three sets of model parameters are presented in Fig. 9. The measured and calculated closure rates after 37 years are also given in this Figure. Fig. 10 shows the development of volumetric strains near the gallery surface for the different models. A comparison of the calculated (with equation (11)) and in situ permeability distributions measured by Häfner et al., [3] is presented in Fig. 11. The numerical prediction of the "Model 1" agrees quite well with the measurement near the gallery surface, but it seems to overestimate the permeability at a distance larger than 0.5 m.

The measured minimal stresses around the gallery and calculated minimal (radial) stresses are given in Fig. 12. The good agreement between the model calculation and the measured data confirms that the current model can predict stress distribution around the gallery with an acceptable accuracy.

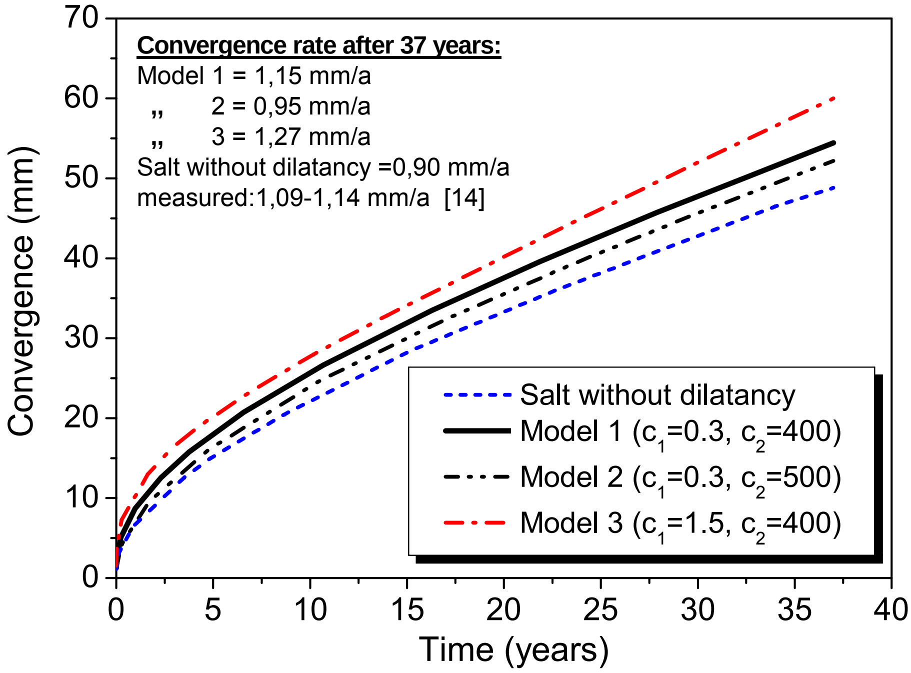

Fig. 9: Gallery convergence calculated for different model parameters and the measured and calculated closure rates 37 years after excavation

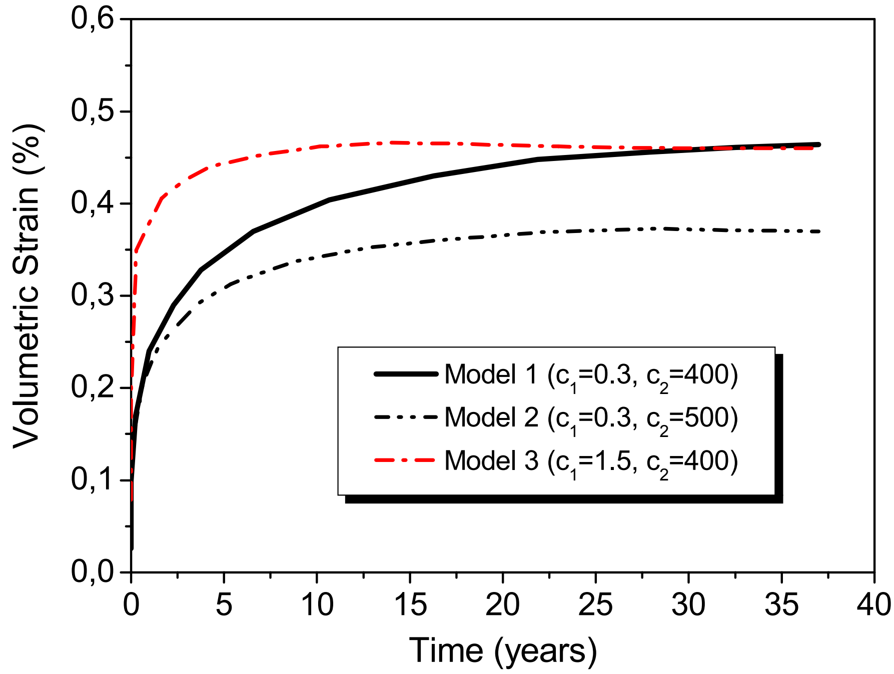

Fig. 10: Model prediction of volumetric strains in rock salt at 5 cm distance from the gallery surface

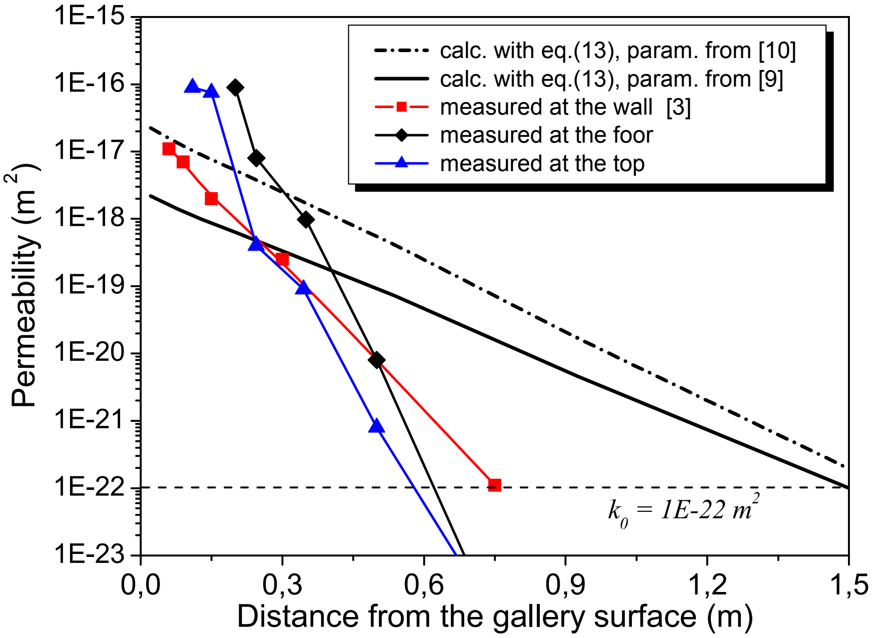

Fig. 11: Comparison of the calculated and measured distribution of rock salt permeability 37 years after excavation

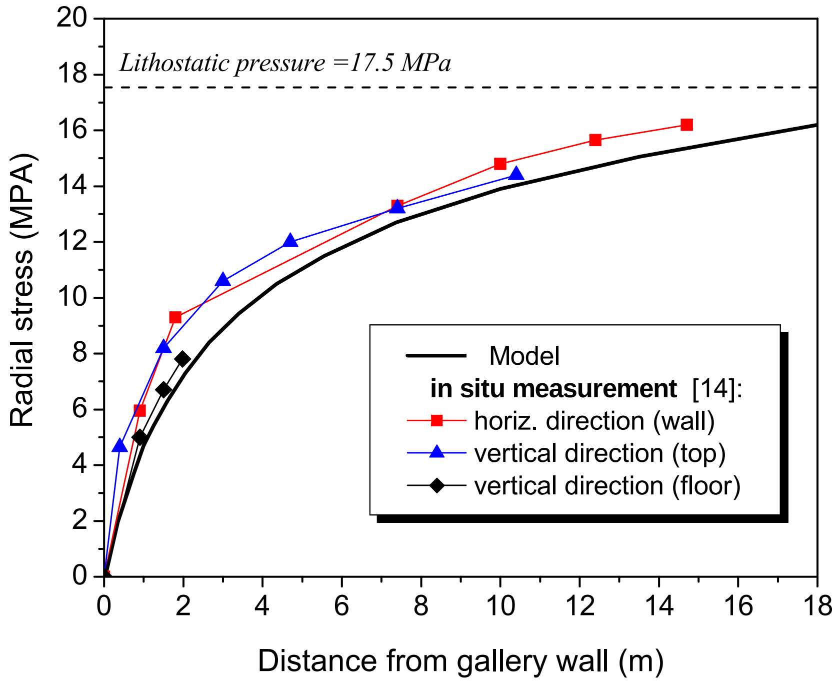

Fig. 12: Comparison of the measured and calculated minimal stresses 37 years after excavation

For illustration, Fig. 13 shows the distribution of calculated displacements, effective stress, minimal stress, and the volumetric strain in the entire model domain 37 years after excavation. It can be seen that the stress field around the gallery will be disturbed in entire model domain due to the creep behaviour of rock salt, but the extension of the damage zone reaches less than 1 m beyond the gallery surface.

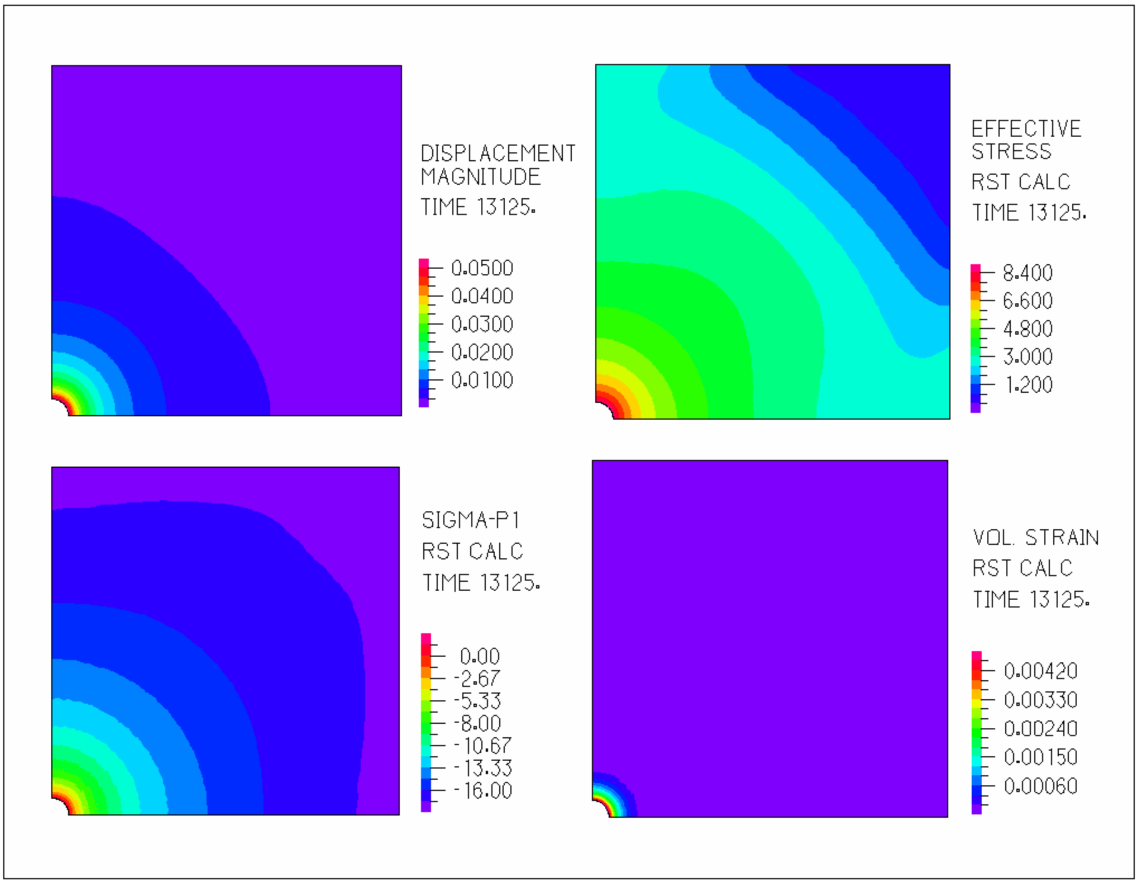

Fig.13: Distribution of displacement, effective stress, minimal stress, and volumetric strain 37 years after excavation

5 Conclusions

A constitutive model for rock salt that permits to describe the development and evolution of the EDZ around the excavations has been implemented in the numerical codes available. Several laboratory experiments have been analysed numerically to gain confidence in the proposed model. At the moment, the calibration of the model parameters is limited by too few reliable triaxial transient creep tests. Further numerical simulations of long-term creep tests will be required to make an overall evaluation of the proposed constitutive model.

Nevertheless, the ability of this model to predict the damage zone around a 37 year' old gallery has been tested. The comparison of numerical results (i.e. stress development and permeability of the rock salt around the gallery) and in-situ measurements indicates that the implemented constitutive model with material parameters fitted to laboratory data works accurately and efficiently.

In the next project phase, the numerical analysis of the development and evolution of EDZ in the near field of a disposal drift in a repository will be performed taking into account the thermal load and the supporting effect of the backfill material.

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