Numerical Analysis of Long–Term Thermomechanical Behavior of Repository Structures

Alexandra Pudewills

Forschungszentrum Karlsruhe GmbH, Institut für Nukleare Entsorgung, 76021 Karlsruhe, Germany

ABSTRACT

During the last decade, several repository concepts were developed for the disposal of high-level radioactive waste from reprocessing and spent-fuel elements in deep salt formations. The elevated temperature in the disposal area and the induced thermomechanical effects have a considerable influence on the long-term safety assessment of such a waste repository. For this purpose, laboratory studies, large-scale in situ experiments, and numerical modeling in order to predict the thermomechanical phenomena in the near and far fields of the repository are performed. This paper summarizes the current state of knowledge concerning the numerical simulation of the thermomechanical effects in the near field of a conceptual repository for disposal of highly radioactive burnt-out spent fuel. The work includes, in particular, the modeling of the temperature fields, thermally induced closure of the underground openings followed by the consolidation of the backfill, and the resulting stresses in the surrounding salt formation. To perform this task, finite element codes containing a set of time- and temperature-dependent constitutive models are used. In a first step the validation of the numerical models and the constitutive equations available for rock salt and backfill material were demonstrated by comparison of calculated results and measured data of a large-scale in situ test. On the basis of these results, the predictive calculations for an emplacement drift in the planned waste repository were performed. The results of the analyses show that under expected repository conditions the volume closure and, hence, the compaction of the backfill are mainly determined by the temperature increase and the lithostatic pressure. Finally, the implications for the post-closure safety evolution are discussed.

INTRODUCTION

Repository concepts for disposal of high-level radioactive waste from reprocessing and spent-fuel assemblies are based on multiple barriers for protection of the environment against the radioactive nuclides. According to these concepts, the containers with heat generating radioactive waste will be placed in vertical boreholes or long parallel drifts at a depth of about 800 to 1000 m below the surface in a rock salt formation [1], [2]. The remaining void space between the containers and host rock will be filled with dry crushed salt. It is expected that in response to the thermally induced creep closure of the excavations the backfill material will compact sufficiently to serve as an efficient seal for the radioactive waste. The performance assessment of such nuclear waste repositories in rock salt requires laboratory tests, field experiments, and the use of adequate numerical models to predict the long-term thermomechanical effects in the near and far fields of the repository. The numerical reliability of the calculations and the predictive capabilities were demonstrated in international benchmark activities and also by comparison with results of the *in situ* heater tests [3].

The scope of this paper is to give an overview of the actual repository concepts focusing on long-term thermomechanical phenomena related to the emplacement of heat-generating waste. This includes numerical modeling of the temperature fields, thermally induced closure of the openings following by the consolidation of the backfill, and the resulting stresses in the surrounding salt. With regard to the behavior of backfill material, the reduction of the porosity and the increase of the pressure on the waste containers were estimated.

The FAST-BEST code, based on the coarse mesh method [4], [5] and specifically developed for studying the drift disposal, was used to predict the temperatures. This program includes temperature-dependent material models for rock salt and crushed salt. The material model for crushed salt takes into account a compaction-dependent thermal conductivity. For the thermomechanical analyses, two finite element codes have been used. One is the general-purpose code ADINA [6] which was extended to investigate the creep compaction of a loose backfill material [7], and the other one is the special-purpose code MAUS [8] which also includes suitable material models for rock salt and crushed salt.

As an illustration of the capability of these codes of solving such complex problems and as a validation of the assumed material models, the numerical simulation of the large-scale *in situ* test TSDE, (**T**hermal **S**imulation of **D**rift **E**mplacement) performed in the Asse salt mine [9], [10] will be used as an example.

Based on the experience gained from the evaluation of this *in situ* test, predictive calculations were carried out for an emplacement drift in the planned repository. The results of the analyses show that under expected repository conditions the volume closure and the compaction of the backfill are mainly determined by the temperature increase and the lithostatic pressure. The porosity of the backfill material will be reduced considerably after few years. With time, the compaction pressure in the backfill increases and therefore supports substantially the rock salt around the drift, and a relevant relaxation and redistribution of stresses in the pillar takes place.

REPOSITORY CONCEPTS

During the last decade the research and development program on direct disposal was focused on a “dual-purpose” repository accommodating both high-level radioactive waste from reprocessing and spent-fuel assemblies [2]. Concerning the disposal concepts, two emplacement techniques were investigated, namely the borehole emplacement and drift emplacement. This paper deals with the drift emplacement concept only.

In a repository designed for drift emplacement, the waste is disposed of in large self-shielded containers (POLLUX casks) which will be placed horizontally on the floor of drifts. In order to utilize the volume in a salt dome efficiently the drifts have to be excavated at three different horizons between 870 m and 1170 m with 150-m distance between two consecutive horizons. Immediately after emplacement, the drifts are backfilled with dry crushed salt. The emplacement panels are bordered by two parallel access drifts as illustrated in Figure 1. At the time of emplacement, the heat generated in a cask will be approximately 7.5 kW, depending on the interim storage period. The cask is 5.5 m long, has a diameter of 1.5 m and weighs ~65 t in its loaded state. The emplacement drifts are 3.5 m wide, 4.0 m high, and about 200 m long and will be excavated into the emplacement panels at a distance of 17 m from each other.

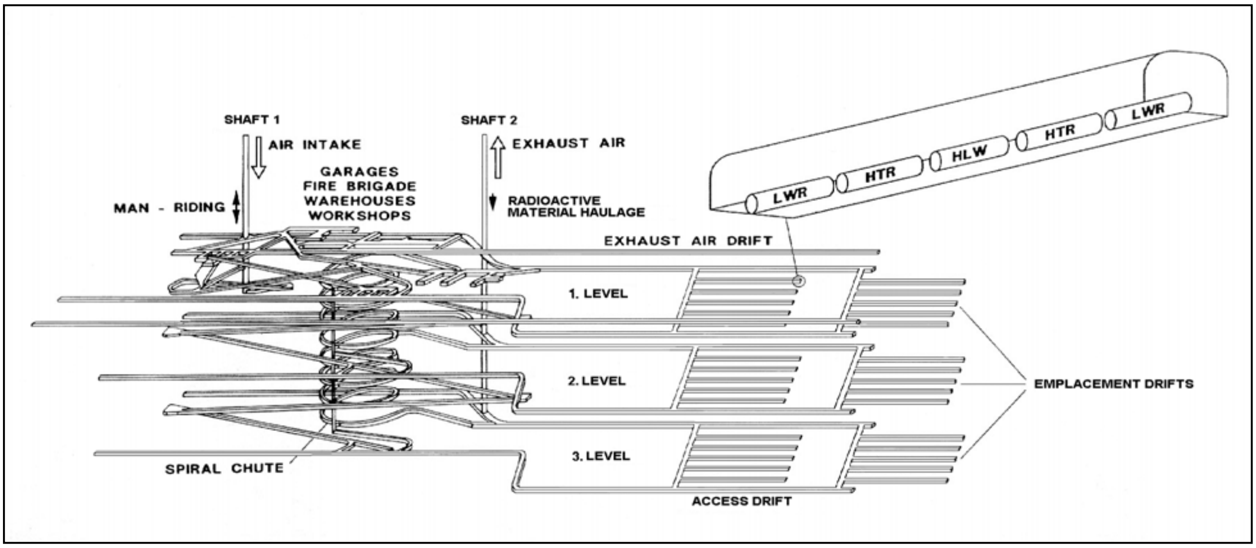


Fig. 1 Three-level drift repository concept (source: Ref. [2])

CONSTITUTIVE MODELS AND THERMOMECHANICAL PROPERTIES

Rock Salt

The thermomechanical behavior of rock salt was described in the finite element analysis by a thermoelastic material model with temperature-dependent steady state creep. According to this model, the total strain rate is given as the sum of elastic, thermal and steady state creep rates. With regard to the waste repository conditions, the long-term steady state creep deformation ought to be considered the most important part of the constitutive behavior of rock salt. This constitutive relation governing the creep deformation of rock salt was proposed by Wallner et al. [11]. The effective creep rate is given by:

$$\dot{\varepsilon}_{ef} = A \, \sigma_{ef}^{5} \exp(-Q/R/T) \tag{1}$$

where

$\dot{\varepsilon}_{ef}$: effective creep strain rate [1/s]

σ_{ef} : effective stress [MPa]

T : temperature [K]

A = $2.06\ 10^{-6}$ $MPa^{-5} s^{-1}$;

Q = 54.21 kJ/mol;

R : universal gas constant, $8.314\ 10^{-3}$ kJ/mol/K

A strength criterion to determine whether or not the rock salt has failed was considered in the numerical modeling. The criterion given by Diekmann et al. [12], was assumed to be:

$$\tau_f = b\,|\,\sigma_m\,|^{\,p} \qquad (2)$$

where:

τ_f : predicted shear stress at failure [MPa]

σ_m : mean stress [MPa]

b = 2.329 and p =0.747 (material constants)

and a safety factor (FS) is defined by the ratio of the current value of the octahedral shear stress ($\tau = \sqrt{2/3}\ \sigma_{ef}$) to the predicted shear stress at failure:

$$FS = \tau / \tau_f \qquad (3)$$

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.

The thermoelastic properties used in the numerical analysis were obtained from reference [13]. Table 1 presents these values together with the properties of crushed salt. The thermal data used for the calculation of the time-dependent temperature fields were assumed to be a function of temperature. Table 2 summarizes the thermal conductivity and specific heat capacity of the rock salt and backfill material.

Table 1: Thermo-elastic properties of rock salt and crushed salt

Properties		Rock Salt	Crushed Salt
Young's modulus:	[MPa]	24000	8000
Poisson's ratio:	-	0.27	0.25
Coefficient of thermal expansion	[K]	$4.2\ 10^{-5}$	$4.2\ 10^{-5}$

Table 2: Thermal properties of rock salt and crushed salt

Properties	Rock Salt	Crushed Salt
Thermal conductivity [W/mK]	$\lambda_r(T)$: 6.10 at 0 °C; 5.02 at 50 °C; 4.19 at 100 °C; 3.57 at 150 °C; 3.11 at 200 °C	$\lambda_c(T,\eta) = \frac{\eta}{\eta_o}\lambda_c^o(T) + (1-\frac{\eta}{\eta_o})^m \lambda_r(T)$ $m = 1.1,\quad \eta_o = 0.35$ $\lambda_c^o(T)$: 0.48 at 0 °C; 0.52 at 50 °C; 0.57 at 100 °C, 0.62 at 150 °C; 0.67 at 200°C
Heat capacity [J/kgK]	c = 890	c = 642

Backfill material

The constitutive relation of crushed salt proposed by Hein [14] was adopted. It is based on a viscoplastic formulation and considers both volumetric and deviatoric strain rates under hydrostatic and deviatoric stress conditions. The material parameter values and the functions h_1 and h_2 are derived from extensive triaxial tests performed by Korthaus [15].

$$\dot{\varepsilon}_{ij} = A \cdot \exp^{-Q/R/T} \cdot (h_1 \cdot p^2 + h_2 \cdot q^2)^{n} \cdot (h_1 \cdot p / 3 \cdot \mathbf{1} + h_2 \cdot \mathbf{Sij}) \tag{4}$$

with

$$h_1(\eta) = a / (((\eta_0/\eta)^{c} - 1) / \eta_0^{c} + d)^{m} \tag{5}$$

$$h_2(\eta) = b \cdot h_1(\eta) + 1 \tag{6}$$

where

$\dot{\varepsilon}_{ij}$: tensor of the strain rate
T : absolute temperature
p : mean normal stress
$\mathbf{1}$: unit tensor
q : deviatoric stress invariant
$\mathbf{Sij}$: tensor of the deviatoric stress

η : porosity
η_0 : initial porosity (35%)
Q : activation energy
R : universal gas constant

Material constants:

$A = 1.09 \cdot 10^{-6}$ MPa $^{-5}$ s $^{-1}$;
$Q/R = 6520$ K^{-1};

$n = 2$;
$a = 2.469\ 10^{-3}$;
$b = 0.9$;

$c = 0.1$;
$m = 2.25$;
$d = 0.0003$

THERMOMECHANICAL ANALYSIS OF A LARGE SCALE IN SITU TEST

The in situ experiment TSDE was performed in the Asse salt mine in Germany in order to demonstrate the emplacement technology and to study the thermal and thermomechanical consequences of the direct disposal of spent nuclear fuel in drifts on the rock mass and technical barriers. A further aim was to evaluate the capability of the available codes to simulate the thermomechanical behavior of the backfill and rock salt under representative repository conditions [4]. The test field is located in a rock salt formation at 800 m depth below the surface. Two parallel drifts were excavated with a length of about 75 m. In each test drift three electrically heated casks with a thermal power of about 6.5 kW were emplaced horizontally on the floor (Figure 2). After installation of the heaters and measuring equipment, the test drifts were filled with dry crushed salt. Heating was started in September 1990 and ended in February 1999.

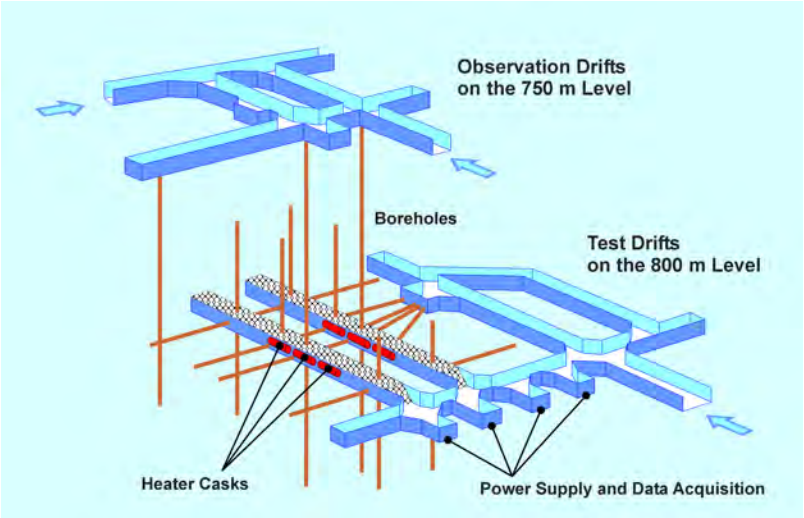


Fig. 2: General view of the TSDE test field [4]

Within the framework of the European project "**BA**ckfill and **M**aterial **B**ehaviour in **U**nderground **S**alt Repositories" (BAMBUS) [3], the development of the temperature in the test field, the thermally induced closure of the drifts followed by the compaction of the backfill, and the resulting stresses in the surrounding salt were studied numerically. Sensitivity studies served to investigate how the assumed material models of crushed salt and rock salt affected the numerical results. The predictive calculations and the comparison with in situ data are raportated in detail in References [16],[17]. Representative results from the numerical simulations only are shown in this paper.

According to the real geometry of the experiment, a three-dimensional finite element model for temperature calculations wes used. A detailed description of this numerical model with the assumed boundary and initial conditions is given in also in Ref. [16] The temperature histories measured and modeled at three characteristic positions through the central cross-section of the test field are shown in Figure 3. The data nearly agree with the calculated temperatures, thus providing confidence in the three-dimensional model used.

To perform the thermomechanical analyses with a reasonable numerical effort, a two-dimensional finite element model was used, assuming generalized plane strain conditions. The model represents a vertical cross-section perpendicular to the drifts at three measuring cross-sections; Two sections located in the zone of maximum temperatures and a section situated in the cooler region. The development of horizontal and vertical drift closure rates measured and calculated for the two cross-sections considered is illustrated in Figure 4. In the heated region the calculation results show an overestimation of the test data. A typical deformed configuration of the backfilled drift is shown in Figure 5. The development of the backfill porosity was not directly measured in the experiment. Generally, the same tendency as for the drift closure presented above can be expected i.e. the porosity reduction will be overestimated by the models used. Due to the temperature-dependent compaction of the backfill and large temperature gradients in the drift, a non-uniform distribution of the backfill porosity over the drift cross- section is expected. Contour plots of calculated porosity distribution in the drift should support this presumption. Figure 6 shows the spatial distribution of the porosity in the drift after 8 years of heating. In the planned post-test project an extensive sampling program with laboratory investigations will be performed to elucidate this presumption.

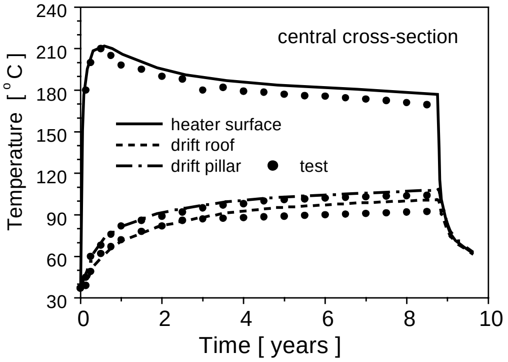


Fig. 3: Comparison of calculated and measured temperatures in the hot cross-section

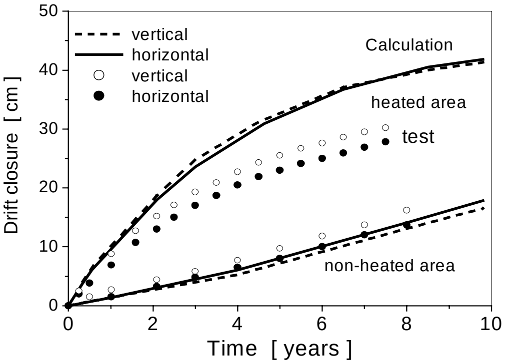
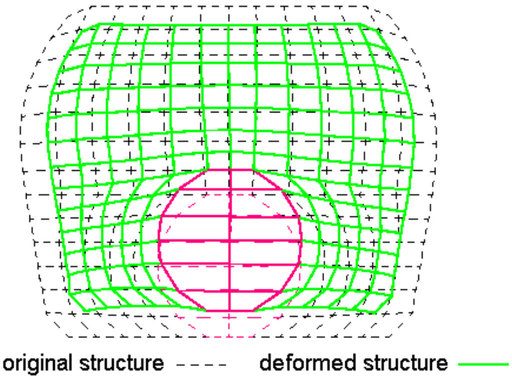


Fig. 4: Drift closure, experimental data and calculation results of two cross-sections

Finally, the thermomechanical results based on the constitutive equations described above lead to some differences between the calculated results and the measurements. The discrepancy could be attributed to uncertainties in the material model of the backfill. Therefore, material parameters obtained from laboratory tests have been adjusted in a parametric study, where the measured and calculated drift closure rates and backfill compaction pressure are matched. Further numerical results of thermomechanical sensitivity analyses [18], [19] suggest that the present deviatoric constitutive model of crushed salt behaves more softly than the crushed salt used in the TSDE experiment. The possible reason for this effect could be a separation of loose salt grains with different sizes during the backfilling process, causing an inhomogeneous distribution over the drift cross-section.



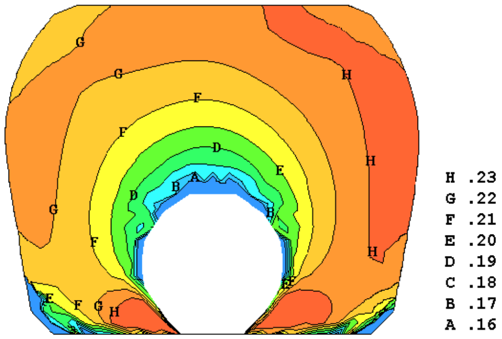


Fig. 5: Deformation of the drift after 8 years of heating in the central cross-section

Fig. 6: Distribution of the porosity after 8 years of heating in the central cross-section

THERMOMECHANICAL CALCULATIONS FOR A DISPOSAL DRIFT

Taking into account the periodic pattern and symmetry of the disposal field, it was also assumed that all disposal drifts in the emplacement panel were excavated and filled with POLLUX casks and crushed salt instantaneously at time zero. A three-dimensional model of a representative portion of the disposal drift were defined for the thermal analysis. In further two-dimensional thermomechanical calculations the temperatures are interpolated from a vertical section passing through the center of the model geometry. A plane strain finite element model was chosen for this thermomechanical investigation. The vertical section right through the center of a POLLUX cask represents only one half of the disposal drift and of the pillar between adjacent drifts.

The numerical simulation started with the calculation of the isothermal convergence and the stress distribution around the disposal drift prior to the emplacement of the POLLUX casks. After about 0.7 years, the temperature development and the of backfill material in the drift were taken into account. The thermomechanical analyses were continued over a period of 50 years. After emplacement of the casks and backfill of the disposal drift, the volume closure and, hence, the compaction of the backfill material are mainly determined by the temperature development and the thermomechanical behavior of the crushed salt.

For a reference case with a pillar width of 12.5 m the histories of the calculated temperatures at three characteristic points are shown in Figure 7. The development of stresses in the backfill material and the decrease of the backfill porosity at two positions in the drift are shown in Figures 8 and 9. Over time, the compaction pressure in the crushed salt increases and becomes large enough to support substantially the rock salt around the drift. These results show that in a repository at a depth of about 870 m the creep rates of rock salt and closure rates will be significantly higher than in the TSDE situ test drifts and that the backfill will be compacted to a porosity of about 1% after ten years of heating.

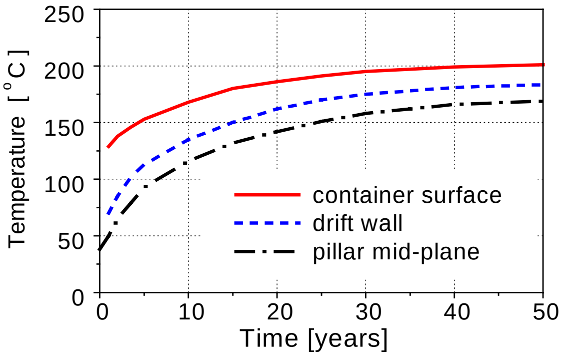
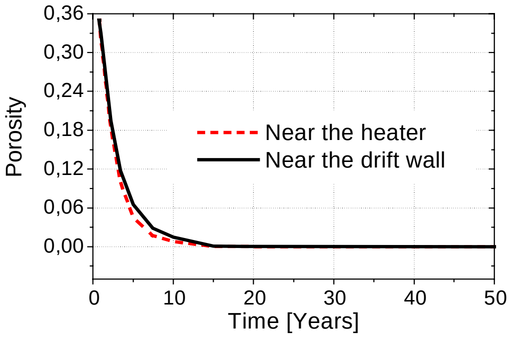


Fig. 7: Calculated temperature histories at different positions



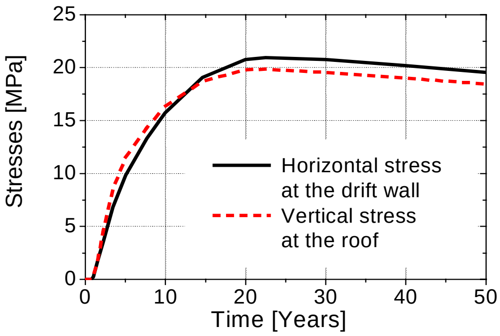


Fig. 8: Development of the backfill porosity **Fig. 9: Development of stresses into the backfill**

The relaxation and the redistribution of stresses in the pillar take place during the first 10 years after the emplacement of the casks. Figure 10 illustrates the spacial distribution of the temperature and mean stress after 5 years of heating. The region in the pillar next to the drift shows highest stress during the operational phase. After emplacement of waste casks and backfilling, the deviatoric stress declines rapidly and tends to become isostatic.

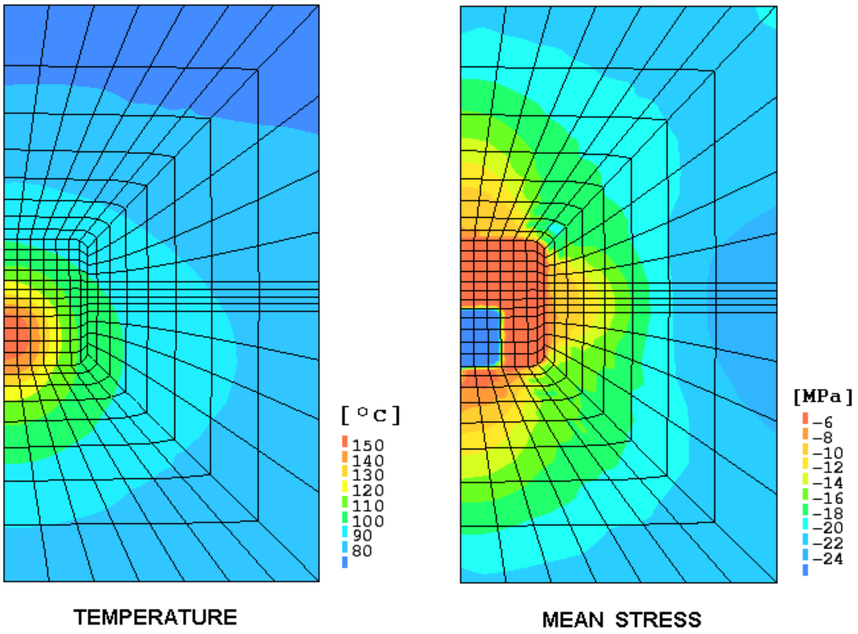


Fig. 10: Temperature and mean stress distributions around in the near field after 5 years

CONCLUSIONS

The agreement between the results of the calculations and the in situ measured values shown that a relatively good prediction can be made of the thermomechanical effects in the near field of the TSDE test with the numerical methods and the material laws used.

Based on these results, the numerical simulation of an emplacement drift in the planned waste repository were performed. Due to thermally induced drift closure, the crushed salt in the drift compacts sufficiently to support the surrounding rock salt and will serve as a seal for the waste casks. Furthermore, the calculations show that in a repository planned at a depth between 870 and 1170 m the rates of rock-salt creep and room closure will be much higher than in the TSDE test drifts and that the backfill will be compacted to a porosity of about 1% after ten years of heating.

High compressive stresses result in the vicinity of the drift during the mining phase. However, the ratio of actual stress to the assumed failure criterion remains less than unity (i.e. no cracks are expected). The results related to the long-term behavior of the disposal drift show that after a few years already, the compaction pressure in the backfill increase rapidly and tends to become hydrostatic, i.e. the effective stress declines and tends slowly towards zero, which means that the surrounding rock salt is relieved.

Acknowledgment: This work has been supported partly by the Commission of the European Communities through the Management and Storage of Radioactive Waste project.

REFERENCES

1. Bechthold, W., Braun, W., Brückner, C., Closs, D., Knapp, U., Papp, R., “Systemanalyse Mischkonzept”, Hauptband, KWA-2190 A1, Kernforschungszentrum Karlsruhe GmbH, 1989.
2. Bechthold, W., Closs, K.D., Knapp, U., Papp, R., “System analysis for a dual-purpose repository”, Final Report, EUR 14595 EN,Brussels, 1993.
3. Bechthold, W., Rothfuchs, T., Poley, A., Ghoreychi, M., Heusermann, S., Gens, A., Olivella, S., “Backfill and Material Behaviour in Underground Repositories for Radioactive Waste in Salt (BAMBUS Project)”, Final Report, EUR-19124 EN, Brussels, 1999.
4. Ploumen, P., Strickmann, G., Winske, P., “Untersuchungen zur Temperaturentwicklung bei der Endlagerung hochradioaktiver Abfälle”, Teil I: Berechnung der zeit- und ortsabhängigen Temperaturfelder, ATW, No.2, pp. 85-91, Feb.1979.
5. Korthaus, E., “Abschließende Verbesserung der vorliegenden Rechenprogramme zur Bestimmung der Temperaturentwicklung”, Abschlußbericht 1980-1982, Vertrag Nr.266-80-7-WASD, EUR 8667 DE, 1983.
6. ADINA, Automatic Dynamic Incremental Nonlinear Analysis, Watertown, MA, ADINA R&D, 1999.
7. Pudewills, A., Krauss, M., “Implementation of a viscoplastic model for crushed salt in the ADINA program”, Computers and Structures, vol. 72, pp. 293-99, 1999.
8. Albers, G., (1983), "MAUS - A Computer Code for Modelling Thermomechanical Stresses in Rock Salt," Computer Modelling of Stresses in Rock, Proc. Tech. Session, EUR9355 EN, Brussels.
9. Bechthold, W., Heusermann, S., Schrimpf, C., Gommlich, G., “Large scale test on in-situ backfill properties and behavior under reference repository conditions”, NEA/CEC Workshop on Sealing of Radioactive Waste Repositories, Braunschweig, Germany, May 22-25, 1989.
10. Droste, J., Feddersen, K. H., Rothfuchs, T., Zimmer, U., “The TSS-Project: Simulation of Drift Emplacement”, Final Report Phase 2, 1993-1995, GRS-127, Gesellschaft für Anlagen- und Reaktorsicherheit mbH, Braunschweig, 1996.
11. Wallner, M., Caninenberg, C., Gonther, H., “Ermittlung zeit- und temperaturabhängiger mechanischer Kennwerte von Salzgestein”, Proc. 4. Int. Congr. Rock. Mech., Vol. 1, Montreux, 1979.
12. Diekmann, N., Hunsche, U., Meister, D., “Über das geomechanische Verhalten von Steinsalz bei erhöhten Temperaturen”, Z. dt. geol. Ges.,: Vol.137, pp.29-46, 1986.
13. Langer, M., “Geotechnical Investigation Methods for Rock Salt”, Bulletin of IAEG, No.25, pp.155-164,
14. Paris, 1982.
15. Hein, H. J., “Ein Stoffgesetz zur Beschreibung des thermomechanischenVerhaltens von Salzgranulat”, Dissertation, RWTH Aachen, 1991.
16. Korthaus, E., ‘Consolidation and Deviatoric Deformation Behaviour of Dry Crushed Salt”, Proc. of 4th Conf. on the Mechanical Behavior of Salt, Montreal, Canada, pp. 365-377, 1996.
17. Pudewills, A., “Thermal Simulation of Drift Emplacement: Temperature Analyses”, Topical Report, FZKA 5955, Forschungszentrum Karlsruhe, 1997.
18. Pudewills, A., “Thermomechanical analysis of the TSS experiment”, Proc. Inter. Congr. Underground Construction in Modern Infrastructure', Stockholm, S, June 7-9, 1998, Rotterdam: Balkema, pp.317-323, 1998.
19. Korthaus, E., “Consolidation behaviour of dry crushed salt: Triaxial tests, benchmark exercise and in situ validation”, Proc. of 5th Conf. on the Mech. Behavior of Salt, Bucharest, Ro., August 9-14,1999, (in print).
20. Pudewills, A., Rothfuchs, T.,“ Thermomechanical Analyses for the TSS-Experiment and Comparison with In Situ Measurements“. The Mech. Behavior of Salt : Proc. of the 5th Conf., Bucharest, Ro., August 9-14, 1999, (in print).