**Thermal-hydraulic-mechanical modeling of a large-scale heater test to investigate rock salt and
crushed salt behavior under repository conditions for heat-generating nuclear waste**

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13 **Abstract**

14 The *Thermal Simulation for Drift Emplacement* heater test is modeled using two simulators for coupled
15 thermal-hydraulic-mechanical processes. Results from the two simulators are in very good agreement.
16 The comparison between measurements and numerical results is also very satisfactory, regarding
17 temperature, drift closure and rock deformation. Concerning backfill compaction, a parameter calibration
18 through inverse modeling was performed due to insufficient data on crushed salt reconsolidation,
19 particularly at high temperatures. We conclude that the two simulators investigated have the capabilities
20 to reproduce the data available, which increases confidence in their use to reliably investigate disposal of
21 heat-generating nuclear waste in saliferous geosystems.

22

23 **Keywords**

24 Heater test, coupled processes modeling, benchmark, heat-generating nuclear waste, rock salt, crushed
25 salt

27 **1. Introduction**

28 The underground disposal of nuclear waste requires the analysis of complex interactions between physical
29 and chemical processes [1-6]. Given the complexity of these inter-related processes and the time scales
30 that need to be considered (typically, thousands or even millions of years for heat-generating nuclear
31 waste), the performance assessment of an underground repository requires that numerical modeling based
32 on suitable tools as well as on state-of-the-art and physically-based knowledge be performed [7].
33 In this research, we focus on sequential approaches to model coupled geomechanics and flow (mass and
34 heat) processes. A detailed description of sequential and fully-coupled formulations for thermal-
35 hydraulic-mechanical (THM) processes modeling, including advantages and drawbacks of each
36 formulation, has been previously provided by different authors [8-16]. In this study, we use two
37 sequential simulators based on the same software, but using two different numerical schemes. The
38 TOUGH-FLAC simulator has been developed at Lawrence Berkeley National Laboratory and is based on
39 the fixed-stress split sequential method [17]. The FLAC-TOUGH simulator has been developed at
40 Clausthal University of Technology and is based on the undrained split sequential method [18]. As their
41 names suggest, both simulators use TOUGH2 [19] to solve the non-isothermal, multicomponent and
42 multiphase flow sub-problem, and FLAC^{3D} [20] to solve the geomechanics sub-problem. These
43 simulators have recently been provided with new features and can now handle finite strains and time-
44 dependent rheology [21]. These enhancements have been motivated by the study of underground disposal
45 of nuclear waste in rock salt formations.

46 Rock salt is a potential medium for the underground disposal of nuclear waste because of several assets,
47 which include its water and gas tightness in the undisturbed state, its very low porosity, its ability to creep
48 and heal technically induced fractures, and its relatively high thermal conductivity as compared to other
49 shallow-crustal rock types [1,2,22-24]. In addition, rock salt is easy to mine and exists underground in
50 large volumes in stable geological areas [25]. The excavated, run-of-mine salt (also referred to as granular
51 or crushed salt) can be used to backfill mined open emplacement zones [26]. Furthermore, worldwide

experience from the salt mining industry is available, and includes construction know-how, long-term behavior of underground excavations in saliferous geosystems, geotectonic inventory of these geosystems and modes of failure mechanisms. Saliferous materials such as salt rock mass (host rock) and crushed salt (backfill) exhibit time-dependent behavior and are known to experience large deformations under certain conditions: salt rock mass creeps under the effect of temperature and deviatoric stresses, and may experience volume changes if the dilatancy boundary is exceeded, or if healing and sealing of micro-fractures occur [6,27-32]; in turn, crushed salt used for backfilling undergoes a reconsolidation process as the excavations tend to close due to the creep of the host rock, which helps encapsulate the waste [33]. During reconsolidation, porosity decreases to low residual values (initial values are normally about 30-40%, and values smaller than 10% are expected in the long-term). In addition, during reconsolidation crushed salt strengthens and its mechanical and flow properties progressively evolve towards the characteristic values of the natural salt host rock [34-36]. It is expected that crushed salt will take an important engineered barrier function in the long-term, thereby reinforcing the geological barrier provided by the natural salt host rock [35,37].

In a recent benchmark exercise, TOUGH-FLAC and FLAC-TOUGH were used to model the long-term performance (over 100,000 years) of a generic salt repository for heat-generating nuclear waste [21,38]. Material-specific characteristics of salt rock mass and crushed salt were implemented into the two simulators. These characteristics are based on experimental evidence as well as on theoretical considerations, and include, but are not limited to, the evolution of rock salt secondary permeability during damage and sealing/healing, and the evolution of crushed salt permeability and thermal conductivity during reconsolidation. A detailed description of all these features can be found in [21]. The results of this benchmark exercise were very satisfactory because the predictions obtained by the two simulators were in very good agreement.

More recently, TOUGH-FLAC and FLAC-TOUGH have been used to model a large-scale underground heater test that was designed to represent reference repository conditions for heat-generating nuclear waste in salt rock mass. In addition to comparing results obtained by the two simulators (benchmark and

code-to-code verification), in this case the numerical results are also compared with available experimental data. This way, the capabilities of the two simulators to predict relevant processes and phenomena can be investigated. This is a fundamental (although preliminary) step to evaluate the suitability of the simulators to study the long-term performance of an underground repository for nuclear waste in rock salt geological formations. An additional target of the simulations performed is to calibrate creep parameters of the natural salt host rock that are difficult to study at laboratory-scale, because they require very small deviatoric stresses, resulting in extremely small strain rates (on the order of 10^{-10} s^{-1}), or, in other words, very long test durations. Moreover, experimental drift closure data have been used to calibrate a parameter set to model backfill setting and compaction, using an existing constitutive law for crushed salt (*cwipp* model implemented in FLAC^{3D} [20]). Compaction behavior of crushed salt is currently not well understood, in particular at small porosities (lower than 5-10%) and also at high temperatures [35,39]. As a result, scarce information is available. Experimental research is underway to gain more insight into these aspects [40,41].

The heater test investigated is the *Thermal Simulation for Drift Emplacement* (TSDE) experiment. It was conducted in the Asse salt mine in Germany in the 1990s to support the development of the in-drift emplacement concept with multiple barriers [37,42]. According to this concept, waste packages containing fuel assemblies are placed on the floor of horizontal drifts, which are subsequently backfilled with crushed salt. The natural salt host rock is the most important barrier, and secondary barriers are provided by the waste packages and the reconsolidated crushed salt backfill. One significant aspect of the TSDE experiment is that it was extensively monitored, using several observation and access drifts, as well as more than 200 boreholes for instrumentation, with sensors scanned every 12 hours. The extensive measurement program included temperature, drift closure, rock deformation, stress evolution and gas generation and transport, among others. Some measuring devices were specially designed for this experiment. Therefore, in addition to evaluating the feasibility of the in-drift emplacement concept, the TSDE experiment provided a vast database on relevant phenomena and processes regarding the host rock, the backfill and also the waste packages. Subsequent analysis of the observations led to an improved

understanding of the behavior of the host rock and the backfill under reference repository conditions for heat-generating nuclear waste, as well as to the development and improvement of constitutive models and computer codes required to predict the aforementioned relevant phenomena and processes [37].

In the TSDE experiment, six electrical heaters were placed in two parallel drifts excavated for the purposes of the experiment in the 800 m level of the Asse mine, in the North-Eastern part of the salt dome. The drifts were excavated in a relatively undisturbed area (Staßfurt Halite of the Zechstein series), and three heaters were emplaced in the central part of each drift. Fig. 1a shows a cross-section of the Asse salt mine and the location of the TSDE experiment, and Fig. 1b shows a view of the two test drifts. Some observation drifts (750 m level) and boreholes can also be seen in the figure.

The dimensions of the drifts, as well as the heat capacity of the electrical heaters, were selected to match the preliminary layout of the in-drift emplacement concept; therefore, the test represented a portion of a typical repository emplacement panel. The heaters were 5.5 m long, had a diameter of 1.6 m and were separated by 3 m along the drift axis. They weighted about 65 t, and their design was based on POLLUX casks for 8 pressurized water reactor (PWR) assemblies. The drifts were about 4.5 m wide and 3.5 m high, and had a length of 77 m. A 10 m wide pillar lay between them. The heaters were emplaced 1.4 years after excavation. Immediately after the emplacement of the heaters, the drifts were backfilled using crushed salt, sieved to retain grain sizes smaller than 45 mm. The heaters were switched on in September 1990, and a constant heat load of 6.4 kW was applied to each heater until February 1999, when the heaters were switched off. The measuring instruments were installed in twenty monitoring cross-sections, not only in the heated area, but also in the non-heated area of the two drifts. Fig. 2 displays a plan view of the two drifts, including instrumented cross-sections.

As compared to previous modeling exercises of the TSDE test [37,43], in this study we include transient, damage and healing processes within the natural salt, and we also account for hydraulic processes.

Performing coupled THM modeling is justified because, although undisturbed rock salt is tight and Staßfurt Halite has low water content [1,2,6,42], an excavation damaged zone (EDZ) is likely to develop around openings, and it could affect flow properties of the host rock (flow of brine, air and heat).

Additionally, during compaction the flow and mechanical properties of crushed salt evolve [34-37]. Most of the previous numerical studies concentrated on thermo-mechanical analyses due to the dominant influence of heating, and its effect on the mechanical response of the host rock and the backfill. Those studies were one-way coupled (from heat flow to mechanics) or two-way coupled, depending on the computational resources available. The improvement in computational capabilities in recent years has made it possible to perform more demanding simulations, yielding a more accurate representation of the systems modeled. The THM simulations presented in this paper are two-way coupled, and account for material-specific characteristics of salt rock mass and crushed salt [21,44]. Due to the real geometry of the experiment, a three-dimensional (3D) representation has been selected for the coupled THM analysis. The need for a 3D configuration was pointed out previously, at least for the computation of the temperature field [37]. Moreover, local effects between heaters cannot be captured in a 2D plane strain approximation. As compared to past studies by the authors [45,46], here we present more complete simulation results, and we present recent inverse modeling work performed to obtain a parameter set for backfill compaction (*cwipp* mechanical model).

In this paper, we first describe briefly the two simulators used. Then, we provide information on the model defined to represent the TSDE configuration, and we explain the modeling sequence and set-up. Later, we present the most significant results obtained and we compare them with experimental data. The calibration of crushed salt parameters (*cwipp* model) is then discussed. This calibration has been performed using iTOUGH2, linked to the PEST protocol [47-49]. Overall, the results obtained from the two simulators are in very good agreement with each other, and also with available experimental data. This finding increases confidence in the potential of both TOUGH-FLAC and FLAC-TOUGH to reliably predict the response of a salt-based repository for heat-generating nuclear waste.

2. Materials and Methods

2.1. Sequential simulators

The simulators TOUGH-FLAC and FLAC-TOUGH are based on the same software: TOUGH2 for heat and multiphase fluid flows [19], and FLAC^{3D} for geomechanics [20]. The flow and geomechanics sub-

problems are solved sequentially (i.e., there are two systems of equations, one for flow and one for geomechanics). Relevant information (e.g., pore pressure, temperature, strain) is transferred between the two codes via intermediate files [10]. This procedure has been selected because the source code of FLAC^{3D} is not available to users. The two simulators benefit from the strengths of the two codes on which they are based, namely, the possibility to model non-isothermal, multiphase and multicomponent (here, water and air) flow, and also the ability to model different rock mechanical responses (FLAC^{3D} has a large library of constitutive models), including time-dependent rheology and large deformations. TOUGH2 is well structured and changes in the source code are not very time-consuming, and FLAC^{3D} provides the user with a capability to implement user-defined constitutive models using plug-in dynamic link libraries, written in C++. An illustrated description of TOUGH-FLAC and FLAC-TOUGH can be found in [21].

The main difference between TOUGH-FLAC and FLAC-TOUGH is that they are based on two different algorithms to sequentially solve the flow and geomechanics sub-problems. TOUGH-FLAC is based on the fixed-stress split sequential method [50]. In this method, the flow sub-problem is solved first in the sequential scheme, using an explicit evaluation of the mean total stress. TOUGH2 is the master code of TOUGH-FLAC, and it moves the simulation forward in time once convergence has been reached in each time step (Newton-Raphson method). FLAC^{3D} is called once per flow time step, and after updating the total stress tensor in each grid-block with pore pressure and temperature changes transferred from TOUGH2, it runs in drained conditions to reach a new state of mechanical equilibrium. Then, relevant information (stress, strains and geometry) is transferred to TOUGH2 in order to compute a new flow time step (accounting for mechanically-induced changes in porosity, permeability and capillary pressure), and this process is repeated sequentially. In contrast, the FLAC-TOUGH simulator has been originally implemented based on the undrained split method [51]. In this method, the geomechanics sub-problem is solved first in the sequential scheme, assuming that fluid mass and temperature remain constant. Pore pressure changes due to volumetric deformation are computed according to the procedure described in [51]. The pore pressure induced by mechanical deformation is transferred to TOUGH2 every time the

coupling is made. Likewise, mechanically-induced changes in porosity and permeability are also transferred, as well as geometry (large strain mode). Starting from this state, TOUGH2 solves the flow sub-problem (mass and heat balances) and computes new pore pressures and additional variables to reach thermo-dynamical equilibrium (temperature, saturations). These new primary variables are transferred to FLAC^{3D} in order to compute the new state of mechanical equilibrium, and the process is repeated sequentially. To reduce computational cost, at present two different sequential methods are available in FLAC-TOUGH. In both methods, FLAC^{3D} is the master code and sequentially (e.g., after each 1000 mechanical creep iteration steps) calls TOUGH2 as a slave code. The first approach, based on the sequential undrained split method, is very computational cost intensive because the necessary FISH-functions in FLAC^{3D} used for updating pore pressures are not parallelized, and called in every FLAC^{3D} iteration step. To reduce the amount of FISH-functions calls, in the second approach the pore pressure is kept constant during the mechanical simulation part, and updated with the overall deformation increment occurring between two consecutive TOUGH2 calls at the end of the mechanical simulation part. This second approach may be seen as a mixture of the undrained split and the drained split methods. The numerical results shown in this paper are obtained using the faster second coupling scheme approach. A recent feature of the two simulators is related to the update of the mesh in the flow sub-problem as finite strains are computed in the geomechanics sub-problem (e.g., due to compaction, consolidation, creep). This feature is also available for 3D domains. The Voronoi partition is recalculated using the software library Voropp [52], and new geometrical data are transferred to TOUGH2 through a text file. These data include: volume of grid-blocks, common interface area between two adjacent grid-blocks, distances from centroids to common interface area and cosine of the angle between the gravity vector and the line linking two neighbor grid-blocks. In the current approach, the centroids of the deformed geomechanics mesh are transferred from FLAC^{3D} to Voropp, which computes the corresponding Voronoi tessellation. The flow mesh is updated every time maximum local strains exceed a preset value, typically 2-5% [53]. Some views of the discretizations used in flow and geomechanics in our simulations are presented in the next section.

2.2. Model description

According to the geometry of the TSDE experiment (see Figs. 1 and 2), we have prepared a 3D model of half of one drift, with two symmetry planes: one at $X=0$ (across the pillar between the two test drifts) and one at $Y=0$ (across the central cross-section of the drifts). Our model is 100 m wide, 200 m high and 38.5 m deep. Fig. 3 shows some views of the initial (i.e., non-deformed) discretization used in geomechanics, including important dimensions. In Fig. 4, some views of the corresponding Voronoi partition are displayed. All external planes are no-flow boundaries. Additionally, the displacement is blocked in the normal direction to those planes. The mesh has 85,870 elements.

Based on available information [42], we assign an initial stress field of 12 MPa to the host rock (isotropic). The initial pore pressure within the host rock is lithostatic, and the initial temperature is 36.4 °C.

Table 1 lists relevant flow and mechanical parameters of the host rock and the crushed salt. These parameters are based as much as possible on available published data [37,54-56]. We highlight that, apart from the grain density, the linear thermal expansion coefficient and the relative permeability parameters, these properties evolve during the simulation as detailed in [21,44]. For code-to-code verification and benchmark purposes, the functions controlling the evolution of properties are the same in TOUGH-FLAC and FLAC-TOUGH, i.e., only the numerical scheme is different (see section 2.1). As compared to [21,44], here the only difference is the model used for the evolution of thermal conductivity. Based on information from the BAMBUS project [37,42], for the host rock (natural salt) we use

$$\lambda_{\text{salt}} = 6.138 - 2.248 \cdot 10^{-2} T + 3.627 \cdot 10^{-5} T^2 + 1.0 \cdot 10^{-9} T^3 \quad (1)$$

with λ_{salt} [$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$] and T [°C]. For the crushed salt, we use

$$\lambda_{\text{crushed salt}} = \max[\lambda_{\text{crushed salt}}, 0 + 1 - \phi] \lambda_{\text{salt}}, 0.8 \quad (2)$$

where ϕ [-] is the current crushed salt porosity, ϕ_0 [-] is the initial crushed salt porosity, $m=1.1$, λ_{salt} [$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$] is given by Eq. (1), and $\lambda_{\text{crushed salt}}$ [$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$]. Moreover,

$$\lambda_{\text{crushed salt}, 0} = 4.758 \cdot 10^{-1} + 8.532 \cdot 10^{-4} \phi + 1.048 \cdot 10^{-6} \phi^2 - 2.222 \cdot 10^{-9} \phi^3 \quad (3)$$

where $\lambda_{\text{crushed salt},0}$ [$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$] and T [$^{\circ}\text{C}$].

As for the electrical heaters, we assume standard properties of stainless steel and linear elasticity. The flow and mechanical properties used for steel are kept constant during the simulation. In agreement with information from the experiment [42], we apply the heat load to the inner part of the heaters, as shown in Fig. 5. The heat load of each heater (6.4 kW) is distributed proportionally to the volume of the grid-blocks used as heat sources.

From the flow point of view, we model two-phase flow of water and air, as well as heat flow. TOUGH2 equation-of-state (EOS) 3 has been used. In TOUGH-FLAC, diffusive mass transport of vapor and air is modeled with coefficients that depend on pressure and temperature [57], and tortuosity effects are accounted for using the Millington and Quirk model [58]. Diffusive flow is for now not considered in FLAC-TOUGH (i.e., advective mass transport is common to both simulators, but diffusion is only considered in TOUGH-FLAC). In both codes, heat flow occurs by conduction and convection.

The mechanical response of the natural salt is described using the *Lux/Wolters* constitutive model, which allows modeling elastic, visco-plastic, damage and healing processes characteristic of rock salt [1,6,59-64]. This state-of-the-art constitutive model has been used to satisfactorily reproduce field and experimental data and has been implemented in FLAC^{3D} as a user-defined model. The total strain rate tensor reads

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^{vp} + \dot{\epsilon}_{ij}^d + \dot{\epsilon}_{ij}^h \quad (4)$$

where superscripts e , vp , d and h stand for elastic, viscoplastic, damage, and healing, respectively. A detailed description of the constitutive model *Lux/Wolters* is given in [64]. The Appendix A of this paper describes the influence of temperature on the rock salt creep deformation, and also damage/dilatancy processes, healing/sealing, and yield and potential functions of constitutive terms. It is important to mention that all the components of the strain rate tensor defined in Eq. (4) take a damage-induced reduction of the load-bearing cross-sectional area into account, in accordance with a previous study [65] (this way, the load-bearing cross-sectional area is the original area multiplied by $1-D$, where D [-] is a

damage parameter [6]). The parameters of the *Lux/Wolters* model used in this research have been determined from the interpretation of experimental results [66]. As will be explained in section 3, three parameters that describe Maxwell viscosity (stationary creep) have been adjusted to the available experimental data of the TSDE test, because their correct determination at laboratory-scale requires very long test durations.

For the crushed salt, we use a modified version of the *cwipp* model implemented in FLAC^{3D} [20,21,34,67]. The main characteristic of the *cwipp* model is that it allows modeling time-dependent volumetric strain changes. While density is not allowed to decrease in the *cwipp* model during reconsolidation (i.e., density is a monotonically increasing function), it honors the volumetric strain evolution in our modified version (only difference with the original model). The total strain rate tensor reads

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^{vc} + \dot{\epsilon}_{ij}^{vs} \quad (5)$$

where superscripts *e*, *vc* and *vs* stand for elastic, viscous compaction and viscous shear, respectively (see section 4 and Appendix B for a description of these terms). For our simulations, we initially used parameters available in the literature [20,68]. Then, in order to achieve a better match of experimental stress data, the parameters of the compaction part were calibrated, as will be explained in detail in section 4. We note that other constitutive laws have been previously used to model the behaviour of crushed salt during the TSDE experiment [42,69,70].

2.3. Modeling sequence and set-up

First, initial equilibrium and drift excavation are modeled. The excavation is assumed instantaneous, and flow during this stage is disregarded. The coupled THM simulations include two parts: (1) the open drift phase, before the emplacement of the electrical heaters and subsequent backfilling of the drifts (1.4 year), and (2) the experiment itself (heating), which lasted 8 years and 5 months.

During the open drift phase, the heaters and backfill are de-activated and the pore pressure is kept constant within the drift at 0.1 MPa. During this phase, the temperature remains approximately constant.

The main purpose of modeling this phase is to investigate the mechanical response of the natural salt host rock (transient, stationary and tertiary creep), including the excavation damage zone. After 1.4 years, the heaters and backfill are activated. The initial porosity of the backfill is 35%, and the initial pore pressure and temperature within the drift are 0.1 MPa and 36.4 °C, respectively [42]. In accordance to the situation sketched in Fig. 2, the extremity of the drift at $Y=38.5$ m is kept hydraulically open at the atmospheric pressure as a boundary condition during the heating phase. This leads to the effect that the pore pressure increase within the crushed salt induced by its compaction as well as by the heating of the included pore fluid is accompanied by a pore pressure decrease induced by an outflow of fluid at the open drift end (ventilation). Therefore, pore pressure cannot increase very much within the drift. Additionally, the drift temperature at this extremity is held at 36.4 °C.

Both during the open drift and heating phases, the mesh used in the flow sub-problem is progressively updated as the mesh used in the geomechanics sub-problem deforms. Depending on the criterion chosen to update the mesh, this operation is performed up to 50 times during the simulations.

Finally, we note that, in order to compute the effective stress tensor (geomechanics sub-problem), we use the saturation-averaged sum of the phase pressures computed in the flow sub-problem. The effective stress tensor, σ'_{ij} [MPa], is defined as

$$\sigma'_{ij} = \sigma_{ij} + \alpha P \delta_{ij} \quad (6)$$

where σ_{ij} [MPa] is the total stress tensor, α [-] is the Biot coefficient, P [MPa] is the pore pressure and δ_{ij} [-] is the Kronecker delta. We note that, in the *Lux/Wolters* model, changes in σ'_{ij} account for damage-induced reductions of the load-bearing cross-sectional area.

3. Results and discussion

Owing to the dominant effect of heating and the significant amount of data available related to thermal processes, the results presented below focus on thermal and thermo-mechanical phenomena.

3.1. Open drift phase: general remarks

Due to a higher number of relevant processes occurring during the heating phase, most of the experimental data and analyses are concentrated on that period. However, a few aspects occurring during the open drift phase should be mentioned. Average vertical convergence rates were about 0.30% per year, and average horizontal convergence rates were about 0.25% per year. Our simulation results are in very good agreement with those rates (results will be displayed in the next sub-section, Fig. 11). In addition, our results suggest that the drift closure rate at the end of this phase is nearly constant. Moreover, due to the stress redistribution induced by the excavation, the dilatancy boundary [1,2,6,27,31] is exceeded, and an excavation damaged zone (EDZ) develops around the drift. It extends about 1.5 m below the drift floor (flat floor), 0.8 m above the roof and 0.75 m beyond the sidewalls. Experimental evidence from the TSDE experiment [37] is in agreement with these EDZ characteristics. In the EDZ, permeability increases up to four orders of magnitude, and porosity reaches values as high as 0.7%. Secondary permeability within rock salt is calculated using a non-linear expression that accounts for dilatancy, effective stresses and their orientation [21,44].

3.2. Heating phase: temperature

Fig. 6 displays the evolution of temperature at several locations within the backfill, in a cross-section containing a heater cask (section B in Fig. 2). The temperature at the heater cask surface is included in the plot; it reached 210 °C five months after the beginning of heating, and it decreased thereafter as the thermal conductivity of the backfill increased (due to compaction), which facilitated the heat flow. The temperature increase was more gradual within the backfill, and significant temperature gradients were measured due to non-uniform compaction (which yields non-uniform thermal conductivity according to Eqs. (2-3)). After about 5 years, temperatures in the heater cask area approached a constant value (160-180 °C at the heater surface), while they continued to increase within the backfill at farther distances from the heater.

Numerical results from TOUGH-FLAC and FLAC-TOUGH are also displayed in Fig. 6, and they are in very good agreement with each other. Moreover, the results reproduce the measurements closely, with highest error at the heater surface. We note that we have performed THM simulations using two different

forms for the evolution of thermal conductivity within the crushed salt. Because most of the heater surface is in contact with crushed salt, the thermal conductivity of the backfill affects temperature at the heater surface. The two forms used have been derived from experimental data [37]. One form is given by Eqs. (2-3), and the other one is given by

$$\lambda_{\text{crushed salt}} = -270\phi^4 + 370\phi^3 - 136\phi^2 + 1.5\phi + 5 \quad (7)$$

where ϕ [-] is the current crushed salt porosity, and $\lambda_{\text{crushed salt}}$ [$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$]. As opposed to Eqs. (2-3), which depend on porosity and temperature, Eq. (7) is only a function of porosity. Both functional forms are displayed in Fig. 7, for porosity and temperature ranges relevant to the TSDE experiment. The simulation results issued from the use of Eqs. (2-3) or Eq. (7) are very similar, showing only some small differences in the temperature evolution of the heater casks during the last years, due to the differences in thermal conductivity of the backfill at small porosities and high temperatures (see Fig. 7).

Fig. 8 shows temperature evolution in additional monitored positions within the backfill: some of them in the heated area (1 m west of sections G2 and B in Fig. 2), and some in the cold area (section E2 in Fig. 2). Again, the results issued from the two simulators are in very good agreement, and they match the measurements quite well. The observed discrepancies, in particular for the curve labelled “2.2 m from floor“, are likely due to local effects: local porosity variations can lead to changes in the computed thermal conductivity, and therefore to different temperatures. But overall, the numerical results reproduce the measured temperatures quite well.

Fig. 9a displays temperature within the rock, in the heated area (section A in Fig. 2), and Fig. 9b displays temperature within the rock, in the non-heated area (section E1). Heat transfer towards the salt rock mass occurs both by direct contact between the heater cask and the drift floor (heated area only), and also through the backfill and the natural salt host rock. As expected, temperature decreases with the increase in depth. While in the heated area temperatures approach a constant value after about 5 years (equilibrium between heat generation and propagation), temperature continues to increase in the cold area (progressive heat propagation). As both figures show, results from TOUGH-FLAC and FLAC-TOUGH are in very

good agreement with each other, and also with experimental data (in the heated area, maximum mismatch corresponds to the heater cask surface).

Finally, Fig. 10 shows rock temperature between the two drifts, in the heated area (section A). In this case, heat flow to the salt rock mass occurs mainly through the backfill. Again, we obtain a very good match of the measurements.

From Figs. 6 and 8-10, we conclude that the temperature evolution and distribution during the TSDE experiment (heated and cold areas) is very well captured by TOUGH-FLAC and FLAC-TOUGH. Also, the two different forms for the evolution of the backfill thermal conductivity (Eqs. (2-3) and Eq. (7)) yield very similar results, with only some differences in the temperature at the heater cask during the last years of heating. We also note that drift ventilation effectively controls pore pressure within the drift, as well as temperature towards the extremity at $Y=38.5$ m.

3.3. Heating phase: drift closure, backfill and host rock porosity, and rock deformation

The drift closure over time is displayed in Fig. 11, for the heated (section G1) and non-heated (section E2) areas. Drift closure is calculated from horizontal and vertical convergence data. Both the open drift and heating phases of the experiment are included in the plot. As the figure shows, the closure rate in the heated area increased significantly (factor of about 12) once heating started. High rates lasted about three months. On the other hand, the closure rate did not change noticeably in the non-heated area when the heaters were turned on. In the heated area, the closure rate decreased progressively over time due to the compaction of the backfill. Indeed, as compaction moves forward, the backfill densifies, stiffens and provides increased mechanical support against the drift walls, thereby reducing the drift closure rate. On the other hand, in the non-heated area the drift closure rate changed smoothly, and during the last five years of heating the vertical and horizontal closure rates were, respectively, 0.26-0.50% per year and 0.26-0.30% per year (values close to those of the open drift phase). In the heated area, closure rates stabilized at 0.5% per year (vertical) and 0.4% per year (horizontal). As the figure shows, results obtained by the two simulators are very similar. Moreover, they fall within the range of experimental measurements. We note that in agreement with experimental evidence from the post-test dismantling

phase [42], drift closure rates are higher at the pillar side of the drift due to higher temperatures at this sidewall. Also, due to the flat floor and the arch-shaped roof, vertical displacement is higher at the floor (uplift).

The numerical results displayed in this paper have been obtained after the calibration of three parameters that control the stationary creep of the natural salt host rock: two of these parameters control the effect of the von Mises equivalent stress on Maxwell viscosity, and the other controls the effect of temperature on that viscosity. These two effects are strongly nonlinear, and numerical results (such as the drift closure displayed in Fig. 11) are very sensitive to them. In addition, the three parameters adjusted are very difficult to measure at laboratory-scale, because they require very small deviatoric stresses, which translate into very small strain rates (on the order of 10^{-10} s^{-1}), and therefore exceedingly long test durations. Consequently, modeling a large-scale, monitored experiment is a useful means for their determination.

Fig. 12 shows the evolution of backfill porosity in the same sections as displayed in Fig. 11. In fact, since backfill porosity was not directly measured during the test, the experimental values displayed in Fig. 12 were recalculated from experimental drift closure measurements [42], yielding an average porosity within a cross-section. For this reason, the comparison between data and numerical results for porosity is only approximate. We recall that high temperature gradients develop within the backfill (see Figs. 6 and 8) and drift closure rates are not uniform; as a result, significant porosity gradients within the backfill are likely, even within a cross-section (heterogeneous compaction) [37]. As the figure shows, during the heating period the average porosity reduced from 35% to 24-25.5% in the heated area, and from 35% to 30-32% in the non-heated area. Therefore, the compaction of the backfill was partial during the test. Using the porosities displayed, maximum values of thermal conductivity reached after 8 years were around $1.5 \text{ Wm}^{-1}\text{K}^{-1}$ according to Eqs. (2-3) (the initial thermal conductivity was $0.8 \text{ Wm}^{-1}\text{K}^{-1}$).

Fig. 13 shows the computed porosity profile within the host rock at the drift contour, at three different times: at the end of the open drift phase, after 4 years of heating, and at the end of the heating phase. As the contours show, porosity increases during heating, particularly in the heated area (thermo-mechanical

damage as defined in [6]), and decreases over time as compaction takes place (development of mechanical support against the drift wall, and subsequent healing/sealing within the host rock). Since compaction is faster in the heated area, in this zone host rock porosity at the end of the test has decreased more than in the non-heated area.

Finally, Fig. 14 shows horizontal displacements within the heated host rock (extensometer data), in the sidewall opposite to the pillar of section A. Experimental data are available until the extensometers failed (after about 7 years of heating). The numerical results obtained by TOUGH-FLAC and FLAC-TOUGH are very similar, and they match quite well the experimental data, with highest mismatch at the wall probably due to a slight mismatch in the primary stress state.

From Figs. 11 and 14, we conclude that drift closure and rock deformation trends are quite well reproduced by the two simulators used in this study.

4. Parameter calibration for crushed salt compaction

4.1. Background

Crushed salt compaction at relevant conditions for heat-generating nuclear waste is under investigation [40,41]. As explained in section 2.2, we model backfill compaction using a modified version of the *cwipp* constitutive model, with a parameter set adapted from previous studies [20,68]. Using this parameter set, the backfill stress evolution during the TSDE experiment could not be modeled satisfactorily, since computed stresses were very small as compared to the experimental data. Experimental backfill stress was measured using hydraulic pressure cells, both in the hot and the cold areas of the drifts [42].

In an attempt to reproduce the measured backfill stress more accurately (provided that stress measurements are correct regarding the measurement procedure), we estimated parameters using inverse modeling.

4.2. Inverse modeling with iTOUGH2-PEST

Using an inverse modeling framework, it is possible to estimate a parameter set that best matches available data regarding the response of a system [47]. In the current case, we try to calibrate the

parameters of the *cwipp* model (compaction part) that best match measured backfill pressure in the hot and the cold areas of the test drifts. The compaction strain rate tensor, $\dot{\epsilon}_{ij}^{vc}$ in Eq. (5), reads

$$\dot{\epsilon}_{ij}^{vc} = \dot{\epsilon}^{vc} \left(\frac{\delta_{ij}}{3} - \frac{s_{ik} \delta_{kj}}{\sigma_{VM}} \right) \quad (8)$$

where δ_{ij} [-] is the Kronecker delta, s_{ik} [MPa] is the deviatoric stress tensor and σ_{VM} [MPa] is the von Mises equivalent stress. The compaction strain rate is given by

$$\dot{\epsilon}^{vc} = \frac{B_0}{\rho} \left[-\exp(-B_1 \sigma'_{ll}) \right] \exp(B_2 \rho) \quad (9)$$

where B_0 [$\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$], B_1 [MPa^{-1}] and B_2 [$\text{m}^3 \cdot \text{kg}^{-1}$] are model parameters, σ'_{ll} [MPa] is the mean effective stress and ρ [$\text{kg} \cdot \text{m}^{-3}$] is the drained density [20]. As density increases during compaction, the elastic parameters (bulk, K , and shear, G , moduli) evolve following a nonlinear empirical expression of the form

$$a = a_{\text{salt}} \exp(a_1 [\rho - \rho_{\text{salt}}]) \quad (10)$$

where $a = \{K, G\}$ [MPa], $a_{\text{salt}} = \{K_{\text{salt}}, G_{\text{salt}}\}$ [MPa] are the elastic constants of the natural salt, and ρ_{salt} [$\text{kg} \cdot \text{m}^{-3}$] is the drained density of the natural salt. Parameter a_1 [$\text{kg}^{-1} \cdot \text{m}^3$] is obtained from the condition that the moduli take their initial values at the initial value of density [20].

In order to perform several runs in a relatively short time (using a forward finite difference approximation, an inversion requires $p+1$ forward runs per iteration, where p is the number of parameters to be estimated [four in our case]), we decided to use a reduced model. Our reduced model comprises the drift only (crushed salt and electrical heaters), and we applied the measured drift closure data (Fig. 11) as a boundary condition along the drift, fixing the displacement normal to the cross-sections at $Y=0$ m and $Y=38.5$ m. We used different closure rates for the hot and the cold areas.

The inversions were performed using iTOUGH2 [47], linked to the PEST protocol [48]. Using this protocol, the algorithms implemented in iTOUGH2 (originally written to perform parameter estimation for the TOUGH2 simulator) are model-independent and can be applied to non-TOUGH2 models, as in

our case (we seek to estimate mechanical compaction parameters). Fig. 15 shows the workflow of iTOUGH2-PEST. More details about the use and theory of iTOUGH2-PEST can be found in [49]. Fig. 16 shows our reduced model (left), including displacement boundary conditions (drift closure rates in the hot and cold areas), and the results of the inversion (right), in terms of experimental and estimated backfill stress. The three curves displayed (stresses at the roof, floor and wall) were considered simultaneously in the inversion. Estimated stress values show systematic trends (i.e., roof data are systematically under-predicted, while floor and wall data are systematically over-predicted), and those trends propagate to the estimated parameter set. This global approach was selected in a first step to determine a tentative parameter set using a reasonable number of runs. In a future step, a more thorough analysis will be undertaken.

The parameters estimated are B_0 , B_1 and B_2 of the *cwipp* model [20], and also the initial Young's modulus of the crushed salt, E_0 . Table 2 shows the initial values of these four parameters (i.e., before performing the inversion), and the best parameter set found through the inversion with iTOUGH2-PEST.

After the inversion on the reduced model, we performed a full 3D THM simulation of the TSDE test, using the parameter set calibrated through the inversion. The results regarding backfill setting are discussed below (other results have already been presented in section 3).

4.3. Computation of backfill stresses

Fig. 17 shows experimental and modeled backfill pressure, both in the hot (section D1) and the cold (section E1) areas. The initial value is atmospheric. Numerical results from the two simulators are in quite good agreement. Maximum differences between measurements and model results are about 0.8 MPa (roof in section D1). We note that the slightly higher stresses obtained by FLAC-TOUGH are the main reason for the smaller drift closure (Fig. 11) and the smaller horizontal displacement at the wall (Fig. 14) computed by this simulator.

Parameter estimation through inverse modeling will be further explored and will be presented elsewhere, since it exceeds the scope of this paper, which deals with the capabilities of two simulators to reproduce relevant processes regarding the disposal of heat-generating nuclear waste in saliferous formations. We

highlight however that it may be difficult to achieve a better match between measurements and model results, due to several reasons. First, backfill compaction is very heterogeneous. Second, drift closure rates likely change progressively over the drift length, although their evolution is not known, and may be affected by local effects such as the presence of a heater cask (during the inversion presented in this paper, two drift closure rates were applied at the drift contour [hot and cold areas]). Third, available drift closure and backfill pressure data were not measured in the same cross-sections, which introduces additional uncertainty to the parameter estimation. Fourth, it may be necessary to further develop the *cwipp* constitutive model, and include a temperature dependency in the compaction part, and/or add other dependencies (experimental evidence at relevant conditions and extensive modeling exercises are necessary to clarify this). To determine the suitability of the current parameter set for other scenarios, in the next sub-section we present experimental and modeling results of an oedometer test.

4.4. Suitability of the estimated parameter set

Using the new parameter set, we have modeled one oedometer test performed on crushed salt cored from one of the TSDE drifts (dismantling phase, see [37] for details). The test was conducted on a cylindrical sample (height of 140 mm and diameter of 280 mm), at a constant temperature of 50 °C. The initial compaction rate applied was $6.9\text{e-}8\text{ s}^{-1}$. This rate was increased to $6.9\text{e-}7\text{ s}^{-1}$ when the porosity was about 19%. Fig. 18 compares experimental data with our numerical results. As the figure shows, there are significant discrepancies, which could be due to the need to further develop the *cwipp* model, and/or to the need to further examine the parameter estimation presented above. The latter will be addressed in the next step of this research.

5. Conclusions

We present coupled thermal-hydraulic-mechanical simulation results of the large-scale *Thermal Simulation for Drift Emplacement* heater test, performed in Germany in the 1990s to investigate the feasibility of underground disposal of heat-generating nuclear waste in rock salt formations, using crushed salt as backfill material. We focus our investigation on the behavior of the natural salt (host rock) and the crushed salt (backfill), and we model both the open drift phase (1.4 year), and the 8.4 years of constant

heat load. The open drift phase is modeled to study the host rock prior to the installation of the heaters and subsequent backfilling. Through the modeling of the TSDE test, our main goal is to evaluate the capabilities of the numerical tools used to reproduce relevant processes and phenomena measured during the experiment, provided that the measurements are correct.

The simulations are performed using two sequential simulators for coupled geomechanics and flow (mass and heat) processes, TOUGH-FLAC and FLAC-TOUGH. Both simulators are based on the same software to solve the flow and geomechanics sub-problems (TOUGH2 and FLAC^{3D}, respectively), but use two different coupling schemes. They can handle finite strains and time-dependent rheology, and include material-specific characteristics of salt rock mass and crushed salt.

The numerical results obtained by the two simulators are in very good agreement with each other, which leads to a code-to-code verification and a successful benchmark exercise. The accuracy of the numerical tools is tested by direct comparison between measurements and simulation results. In terms of temperature, rock deformation and drift closure, our results are in quite good agreement with available experimental data from the test. Regarding backfill compaction and associated setting (i.e., stress increase), drift closure data from the experiment have been used to calibrate parameters of the *cwipp* model (compaction part). For this purpose, we have used a reduced model derived from the full 3D one, consisting only of the crushed salt and the electrical heaters, and we have applied the measured drift closure rate during the heating period as a boundary condition. Through inverse modeling, we have estimated a parameter set. This approach has been selected due to the limited amount of available data regarding crushed salt compaction, in particular at high temperatures. The parameter set obtained has been subsequently used to model the TSDE experiment, and the results are more satisfactory than before the inversion. In order to test the suitability of the current parameter set for other scenarios, we have modeled an oedometer test conducted on crushed salt from one of the TSDE drifts. The results show some discrepancies, which could be due to the need to further develop the *cwipp* model (for instance, model compaction as a function of temperature, or include additional dependencies), and/or to the need to

further explore parameter estimation through inverse modeling. The latter will be addressed in the next step of this research.

The modeling of the TSDE experiment has also led to the adjustment of three parameters that control the stationary creep of the natural salt. These parameters are difficult to study at laboratory-scale because they require very small deviatoric stresses, resulting in very small strain rates and therefore extremely long test durations.

From the overall rather positive direct comparison between measurements and numerical results, we conclude that TOUGH-FLAC and FLAC-TOUGH have the necessary capabilities to reproduce relevant experimental data and to study complex coupled processes in the scenario considered (provided that the measurements available are correct). Although this finding increases confidence in the use of the two simulators to reliably investigate the performance of an underground repository for heat-generating nuclear waste in rock salt formations, we note that at this stage the successful use of these numerical tools to investigate other scenarios is not guaranteed.

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Figure captions

Fig. 1. (a): cross-section of the Asse salt mine, indicating the location of the TSDE experiment; (b): schematic representation of the TSDE test area.

Fig. 2. Plan view of the test drifts and monitoring cross-sections.

Fig. 3. Views of the initial (non-deformed) mesh used in the geomechanics sub-problem. The main dimensions of the model are also shown.

Fig. 4. Views of the initial (non-deformed) mesh used in the flow sub-problem. Only the drift area is displayed. In the first figure, only one column of elements along the Y axis is shown.

Fig. 5. Discretization of the electrical heaters (only half of one heater is shown). The elements in gray are the heat sources during the THM simulations.

Fig. 6. Temperature evolution within the backfill (section B) and at the heater surface. Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 7. Comparison of two empirical expressions to determine the thermal conductivity of compacting crushed salt. Both expressions have been proposed previously [37].

Fig. 8. Temperature evolution within the backfill (filled symbols refer to a section located 1 m west of section G2 and non-filled symbols refer to a section located 1 m west of section B. The curve labelled “12 m from heater” corresponds to the floor in section E2). Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 9. Temperature evolution within the host rock, beneath the floor in (a) section A, and (b) section E1. In section A, temperature at the heater surface is also displayed. Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 10. Temperature evolution within the pillar between the two test drifts (section A). Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 11. Drift closure in the heated area (section G1) and in the non-heated area (section E2). The start of the heating phase is set as a reference time ($t=0$), and also as a reference for drift closure (i.e., during the open drift phase, the drifts are closing). Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 12. Backfill porosity in the heated area (section G1) and in the non-heated area (section E2). Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 13. Host rock porosity around the drift area at three different moments of the THM run (TOUGH-FLAC).

Fig. 14. Horizontal displacement (section A, sidewall opposite to pillar). Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 15. Architecture of iTOUGH2 linked to the PEST protocol [49].

Fig. 16. Reduced model used in the inversion (left) and results (right).

Fig. 17. Backfill stress increase in the heated area (section D1) and in the non-heated area (section E1). In the non-heated area, the oscillations in the experimental data are due to seasonal variations in the pore pressure. Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH simulation results.

Fig. 18. Experimental and modeled results of an oedometer test conducted on a crushed salt sample taken from one of the TSDE drifts.

Table 1. Mechanical and flow properties of the crushed salt and the natural salt.

Property [unit]	Crushed salt	Rock salt
Bulk modulus, K [MPa]	150 ^a	17,390 ^b
Shear modulus, G [MPa]	70 ^a	9450 ^b
Initial Biot coefficient, α [-]	1 ^a	0.003 ^b
Porosity ϕ [-]	0.35 ^a	0.002 ^b
Permeability, k [m ²]	$5.8 \cdot 10^{-13}$ ^a	0 ^b
Initial thermal conductivity (36.4 °C) [W·m ⁻¹ ·K ⁻¹]	0.8 ^a	5.37 ^c
Initial heat capacity (36.4 °C) [J·kg ⁻¹ ·K ⁻¹]	860 ^c	860 ^c
Initial liquid saturation, S_l [-]	0.02	0.5
Grain density, ρ [kg·m ⁻³]	2154	2154
Linear thermal expansion coeff., α_T [K ⁻¹]	$4.2 \cdot 10^{-5}$	$4.2 \cdot 10^{-5}$
Relative permeability functions	Corey	Corey
Residual liquid saturation, S_{lr} [-]	0.05	0.05
Residual gas saturation, S_{gr} [-]	0	0

^a: non-constant value (changes during reconsolidation); ^b: damage- and healing-dependent value; ^c: temperature-dependent property

Table 2. Parameter sets used to model compaction, before and after the inversion (for the latter, significant digits are shown to reflect uncertainty).

Parameter [unit]	Before inversion	After inversion
B_0 [kg·m ⁻³ ·s ⁻¹]	$8.6 \cdot 10^8$	$4.6 \cdot 10^8$
B_I [MPa ⁻¹]	0.195	2.0
B_2 [m ³ ·kg ⁻¹]	$-1.72 \cdot 10^{-2}$	$-2.46 \cdot 10^{-2}$
E_0 [MPa]	182	10.1

Figure 1a

Figure 1b

Figure 2

Figure 3

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9a

Figure 9b

Figure 10

Figure 11

Figure 12

Figure 13

Figure 14

Figure 15

Figure 16

Figure 17

Figure 18