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A systematic strategy for strengthening the reliable prediction of crushed salt constitutive models

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Abstract. Crushed salt will be used as backfill material for openings in a potential high-level nuclear waste (HLW) repository in rock salt. Together with the host rock, the backfill material will provide long-term sealing for isolation of radionuclides. Therefore, the understanding of its behavior and evolution over time is crucial. This paper presents a strategy to improve the predictive quality of constitutive crushed salt models for the long-term safety of an HLW repository. The systematic strategy is developed and applied within the framework of the KOMPASS projects (Czaikowski et al., 2020; Friedenberg et al., 2024) and the currently running MEASURES project (2024–2027). It covers the creation of a reliable experimental database that is subsequently used for model analysis and model development and optimization. The progress of model improvement is indicated by a virtual demonstrator, which represents a generic backfilled drift in rock salt. In its current state, the approach's success is demonstrated by a reduction in bandwidth across the different crushed salt models in the demonstrator results for mean stress at an intermediate porosity range. The work is ongoing, and major achievements will be available at the end of the MEASURES project.

1 The role of crushed salt in the concept of a repository for high-level nuclear waste in rock salt

In siting processes for a high-level nuclear waste (HLW) repository, countries such as Germany, the Netherlands, and the United States consider rock salt to be a potential host rock. Rock salt possesses several favorable properties to isolate the heat-emitting waste and, therefore, the radionuclides from the biosphere, including high thermal conductivity, hydraulic tightness, and viscoplastic deformation properties (Bundesgesellschaft für Endlagerung, 2020). The safety concept for a repository in rock salt is based on a multi-barrier system. This includes the geological barrier (i.e., rock salt), geotechnical barriers (i.e., backfill, crushed salt), sealing elements (e.g., salt concrete), and technical barriers (i.e., waste canister, waste matrix). Technical barriers and sealing elements provide short-term sealing during their designed lifetime. Long-term sealing is provided by crushed salt backfill and rock salt, making the crushed salt's long-term safety function crucial.

Crushed salt backfill possesses favorable properties similar to those of rock salt. As it is a native material derived from the excavation of underground facilities, the compatibility between the host rock and the backfill material is guaranteed. The crushed salt will be compacted over time by creep-driven convergence of the rock salt, reducing its initially high porosity (30 %–40 %) to values comparable to those of undisturbed rock salt (≤ 1 %).

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The compaction process is determined by internal material properties (e.g., grain size and/or grain size distribution, mineralogy, and moisture content) and by the surrounding conditions (e.g., temperature, stress state, convergence rate, and here also moisture content). Therefore, it comprises several thermal–hydraulic–mechanical (THM) coupled processes (Castagna, 2007; Hansen et al., 2015; Svensson et al., 2025; Tounsi et al., 2023). For predicting the evolution of crushed salt's sealing function in the safety analysis of a rock salt repository, understanding the complete compaction process, including the porosity–permeability relationship; adequately describing the processes and their essential influencing factors; and providing a robust, reliable prognosis with validated constitutive models are crucial. For the long-term safety assessment, the point in time at which crushed salt achieves its sealing effect is crucial. Therefore, the timescale of crushed salt compaction is a safety factor.

2 Efforts to advance the process understanding of crushed salt compaction

With the shift in the German safety case due to the Site Selection Act in 2017, crushed salt's role changed from mechanical host rock stabilization to an important geotechnical barrier with hydraulic and mechanical safety functions. As crushed salt research came into greater focus and thermo-mechanical considerations shifted to thermo-hydro-mechanical coupled considerations, new efforts to improve the predictive quality of crushed salt compaction began with the KOMPASS project (Czaikowski et al., 2020). Within the project, methods and strategies were developed to reduce existing gaps in the process understanding of crushed salt compaction. The approach was characterized by a strong connection among the three main topics: laboratory studies, microstructural investigations, and numerical methods. With the KOMPASS-II project (Friedenberg et al., 2024), the activities were continued, and the primary achievements were as follows:

- specification of the KOMPASS reference material, a well-defined and reproducible crushed salt material for generic investigations;
- development of pre-compaction methods and successful production of samples in the short term and under in situ-relevant stresses;
- formulation of a systematic laboratory program addressing the isolated investigation of known relevant factors influencing the crushed salt compaction process;
- construction of an in situ KOMPASS backfill body in the Sondershausen mine due to the collaboration with the SAVER project (Mischo et al., 2024);
- advancement of tools for microstructure investigation methods;
- beginning of the summary of a micro-physical process list combining literature research and own findings;
- performance of the long-term compaction tests according to the designed lab program;
- benchmarking of long-term triaxial compaction tests, including optimization of the models;
- application of a virtual demonstrator for qualitative and quantitative comparison of the models, including modeling variations before and after the validation work based on the new lab data.

Overall, the KOMPASS projects made significant progress in addressing open questions about the long-term safety of a nuclear waste repository in rock salt. However, not all open questions could be addressed within the restricted time, and new important shortcomings were identified (Friedenberg et al., 2024). The main points are as follows:

- The laboratory program is incomplete; factors such as moisture content have not yet been thoroughly investigated experimentally. Furthermore, the numerical simulations indicated a need to extend the ranges of mean stress and porosity investigated.
- The effects of laboratory shortcomings on the numerical extrapolation of laboratory compaction tests to in situ compaction need to be investigated. In particular, sample-to-sample variability must be investigated and, if needed, assessed, as well as lab-to-lab variability (or pre-compaction method).
- Hydraulic properties need to be investigated, especially for the low-porosity range.
- The essential investigation of in situ-compacted crushed salt for quantifying microstructures and the related deformation mechanism is still pending.
- The need for specialized microstructural experiments has been identified.
- The model calibration is incomplete and has to be continued based on the new lab data.

Thus, the project family continues its efforts to improve the understanding and predictability of crushed salt compaction within the MEASURES project (Friedenberg et al., 2025). As presented above, the projects cover a broad range of crushed salt investigations that interact closely with one another. However, the focus of this paper is on the numerical part.

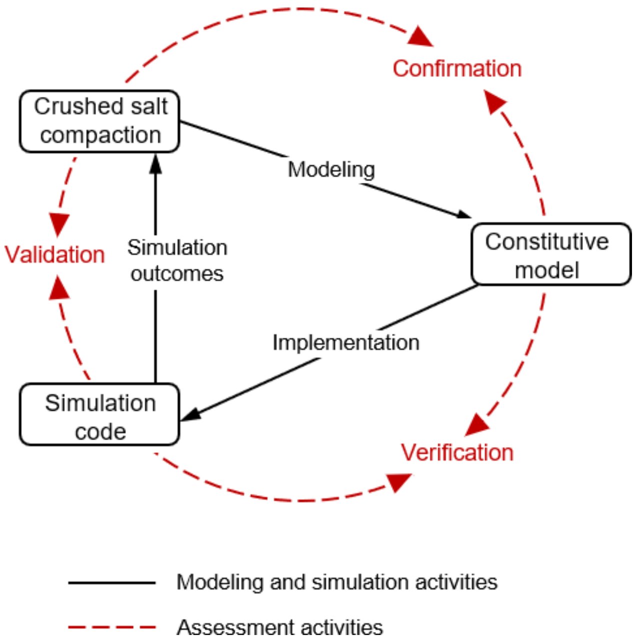

Figure 1. Schematic representation of the modeling, simulation, and assessment workflow for crushed salt compaction. Modified after Thacker et al. (2004).

3 The approach for a systematic improvement of crushed salt constitutive models and their predictions

Within the KOMPASS projects and the MEASURES project, a systematic strategy is being developed to improve existing crushed salt constitutive models and to enhance their predictive quality. Since the amount of knowledge gained during the projects has increased significantly, the strategy possesses some flexibility to react to newly occurring questions.

Figure 1 gives a generalized overview of the modeling, simulation, and assessment workflow for crushed salt compaction. It illustrates the interaction between three core components: (i) the constitutive model, (ii) the simulation code, and (iii) the crushed salt compaction process. Modeling activities link the physical process of crushed salt compaction to the constitutive model, while implementation connects the constitutive model to the simulation code. Simulation outcomes are fed back from the simulation code to the crushed salt compaction process. Assessment activities are shown as a dashed red circular loop encompassing the workflow and include verification of the simulation code, validation of simulation results against experimental or observational data, and confirmation of the constitutive model. Solid black arrows denote modeling and simulation activities.

Figure 1 presents the core modeling and simulation loop underlying crushed salt compaction analyses, including the associated assessment steps. Figure 2 builds on this foundation by illustrating how these elements are implemented and refined within a broader, long-term research framework (e.g., KOMPASS-I, KOMPASS-II, and MEASURES), highlighting the progressive reduction in uncertainties and the improvement in the quality of derived statements. The left-hand side illustrates the application-oriented modeling chain, linking in situ application to numerical simulations, constitutive modeling, and an experimental database, emphasizing the interdependence of experiments and modeling. The central column highlights key scientific and technical quality criteria, including practicability, functionality, accuracy, and transferability, which are to be improved, supported by verification and validation activities. These contribute to the stability, robustness, and suitability of the modeling approaches, ultimately enabling reliable statements close to reality, applicable in retrospective, current, and prognostic contexts. The lower part of the figure outlines the general evolution of methods and projects (from KOMPASS-I to KOMPASS-II and MEASURES) over time and with different resources, alongside the associated reductions in uncertainty and the decreasing need for assumptions and extrapolations. Overall, the presented strategy emphasizes the progressive improvement of quality, robustness, and reliability through systematic experimental design, modeling, and assessment.

The experimental database is built on triaxial compaction tests performed on the KOMPASS reference material. Figure 3 presents the systematic laboratory program that builds the basis for advancing the experimental database. The aim is to isolate known relevant factors influencing the crushed salt compaction behavior in a repository during triaxial compaction tests and subsequently using the data and observed relations for constitutive modeling. To date, the experimental database has grown solely through the performance of laboratory tests as in situ measurements are rare or not applicable. Thus, the presented framework of confirmation, verification, and validation (Fig. 1) applies to laboratory tests and is planned to be expanded to in situ applications in the future.

The in situ investigation is based on the KOMPASS backfill body that was established in 2023 in cooperation with the SAVER and SAVER-2 projects (Mischo et al., 2024). The backfill body is of outstanding scientific and technical relevance as it provides direct insights into the mechanical and hydraulic behavior of crushed salt under in situ conditions. With ongoing monitoring efforts, the long-sought experimental validation of laboratory findings under conditions representative of an actual under-ground nuclear waste repository will be provided.

However, the experimental database includes not only compaction experiments but also microstructural investigations that give insights into the relations between microstructural evidence and deformation mechanisms. The topic of microstructural investigations is broad and not the focus of this paper. For more information, refer to the KOMPASS projects reports (Czaikowski et al., 2020; Friedenberg et al., 2024).

A variety of constitutive models for crushed salt compaction are applied, as shown in Table 1. These models are

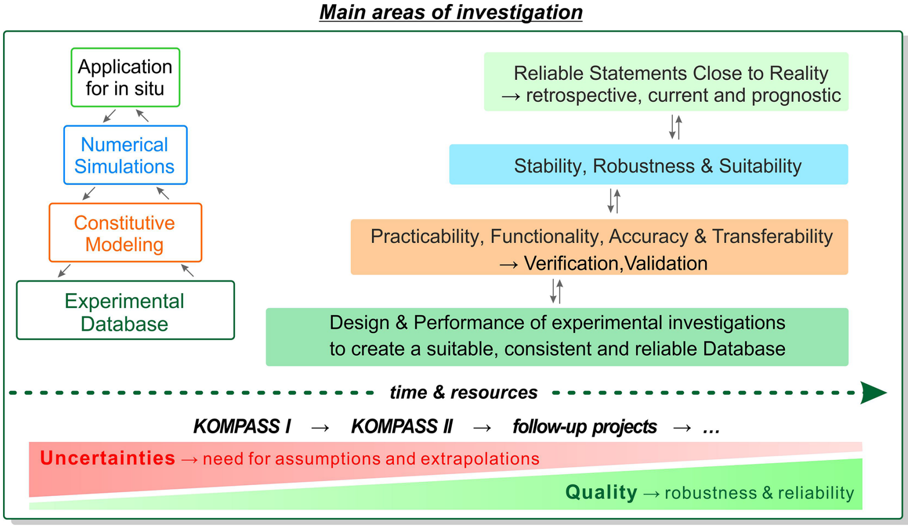

Figure 2. Overview of the main areas of investigation and methodological workflow for the development of reliable simulation-based statements.

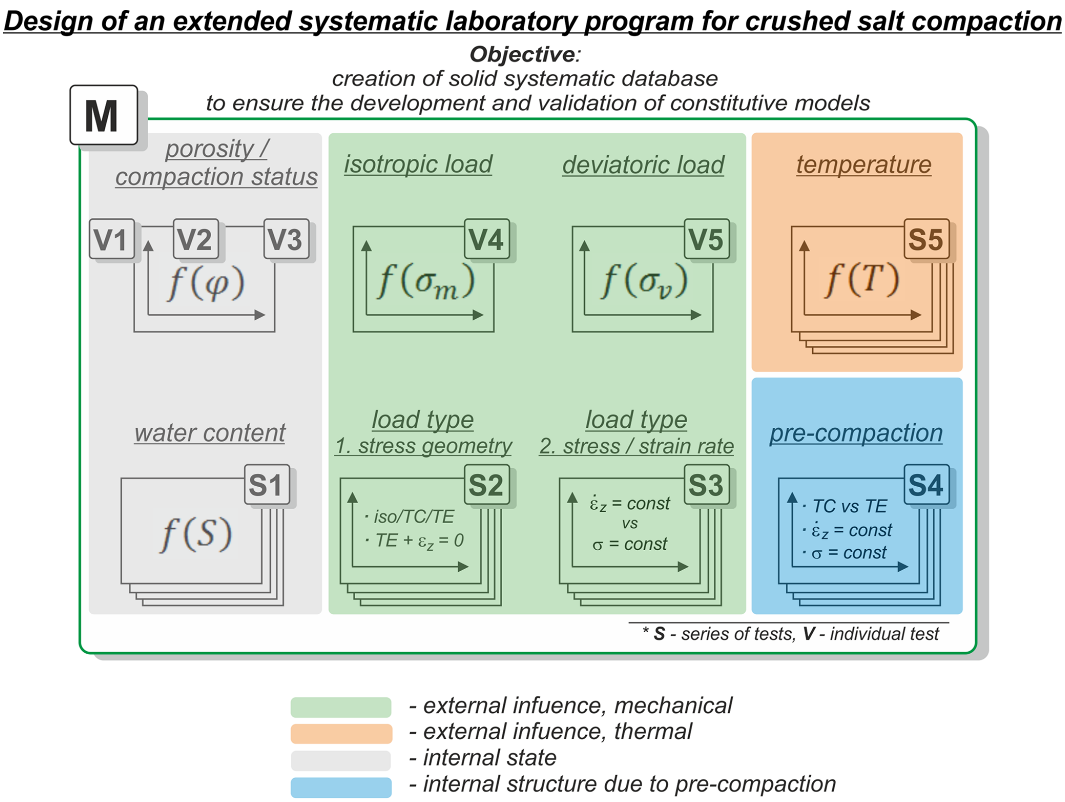

Figure 3. Systematic laboratory program as a basis for building the experimental database in the crushed salt projects.

all in use in the field of repository research; however, there is no constitutive model that is validated against (1) the whole porosity range for crushed salt compaction (especially < 5 %) and (2) all factors or processes influencing compaction (especially moisture). Different constitutive models must be employed, and the results must be compared to build confidence, ensure quality assurance, and ensure robust results. Since there is no complete consensus on formulating constitutive models, uncertainties are captured by using different formulation options to account for many complex physical processes and by using different methods (finite-element method and/or finite-difference method).

Table 1. Overview of constitutive models for crushed salt and simulation codes.

Organization	Constitutive model	Simulation code	Method
BGE-TEC	Hein-Korthaus[a]	FLAC 3D	FDM
BGR	BGR-CS[a]	JIFE	FEM
GRS	CODE_BRIGHT model	CODE_BRIGHT	FEM
IfG	Modified C-WIPP model[a]	FLAC 3D	FDM
Sandia	Callahan model[a]	Sierra/Solid mechanics	FEM
TUC	EXPO-COM[b]	FLAC 3D	FDM

[a] Models are under development or are being updated. [b] Model is newly developed in the framework of the KOMPASS projects.

Model development–optimization is an iterative process performed several times. New triaxial compaction tests deliver new benchmark cases and new information for model optimization. The continuous improvement of the constitutive models is visualized using a virtual demonstrator representing a generic singular backfilled drift in rock salt (Fig. 4a). The virtual demonstrator is envisaged as a tool to visualize and quantify calibration progress and not to compare simulation results with in situ data. After the investigation of each new factor or process is completed, the virtual demonstrator is applied, and the evolution of porosity and mean stress – identified as the most important process variables – is evaluated by comparing the results obtained by different teams. The use of the relatively simple virtual demonstrator ensures that all models reproduce the simplified behavior of rock salt in a consistent manner, such that the only differences between the models arise from the constitutive description of crushed salt. In this way, changes in individual team results and the bandwidth of the predictions associated with the various crushed salt models can be systematically assessed.

The interaction between the laboratory experiments, constitutive model development, and virtual demonstrator is shown in Fig. 4b. Laboratory experiments provide the fundamental data used to confirm and validate constitutive model components, and benchmarking supports consistency checks between different constitutive models. After implementing the constitutive model, the virtual demonstrator enables application-oriented numerical tests, enabling model improvements and assessments under representative conditions.

4 Application

The strategy presented above builds on an iterative approach of adding information, modeling, model development and/or optimization, and application of the virtual demonstrator. The constitutive models from Table 1 are applied to benchmark calculations of triaxial compaction tests. Each benchmark test is followed by model evaluation and if necessary, subsequent model development and/or optimization. Then, the virtual demonstrator is applied to the current state of the model, and the porosity evolution is compared between the models. Afterwards, another benchmark calculation is started, focusing on new information to be added.

At the beginning of the crushed salt investigations (KOMPASS-I project, Czaikowski et al., 2020), the KOMPASS reference material was newly specified, and so no data were available. The models were benchmarked against a triaxial compaction test and compared using the virtual demonstrator. At the end of the KOMPASS-II project, progress was made in the experimental investigation of mean stress, deviatoric stress, temperature, and porosity (as shown in Fig. 3), providing a solid basis for model development and/or optimization. The constitutive models are benchmarked against the triaxial compaction test TUC-V2, as shown in Fig. 5.

The test is divided into five phases (I–V). The main plot shows the temporal evolution of stress components ($\sigma_z =$ axial stress, $\sigma_x =$ radial stress, $\sigma_\mathrm{m} =$ mean stress, $\sigma_\mathrm{v} =$ deviatoric stress) alongside the applied temperature profile (T cell). Stress levels and temperature steps are displayed as stepwise functions over a total duration of more than 750 d. The boundary conditions (B/C) correspond to isotropic and deviatoric loading using Sondershausen rock salt, applied in six levels of mean stress (σ_m), one level of deviatoric stress (σ_v), and three thermal levels. The left panel summarizes the influencing factors investigated in the study. These include porosity (Φ), mean stress (σ_m), temperature (T), and deviatoric stress (σ_v). The bottom row illustrates the measurement relevance of each influencing factor (InF), distinguishing between values obtained from laboratory measurements (green region) and extrapolated ranges required for in situ assessment (orange region). Each subplot displays the corresponding parameter range for InF1 to InF5 and highlights the transition from laboratory-determined data to conditions representative of repository environments.

The early phases of the test focused on mean stress increase and cyclic loading of deviatoric stress, followed by a long steady-state period and subsequently by combined high-temperature and mechanical loading. The experimental design allows systematic investigation of key influencing factors on crushed salt behavior, including mean stress (compaction), deviatoric stress, temperature, and creep. The schematic panels at the bottom illustrate the relationship be-

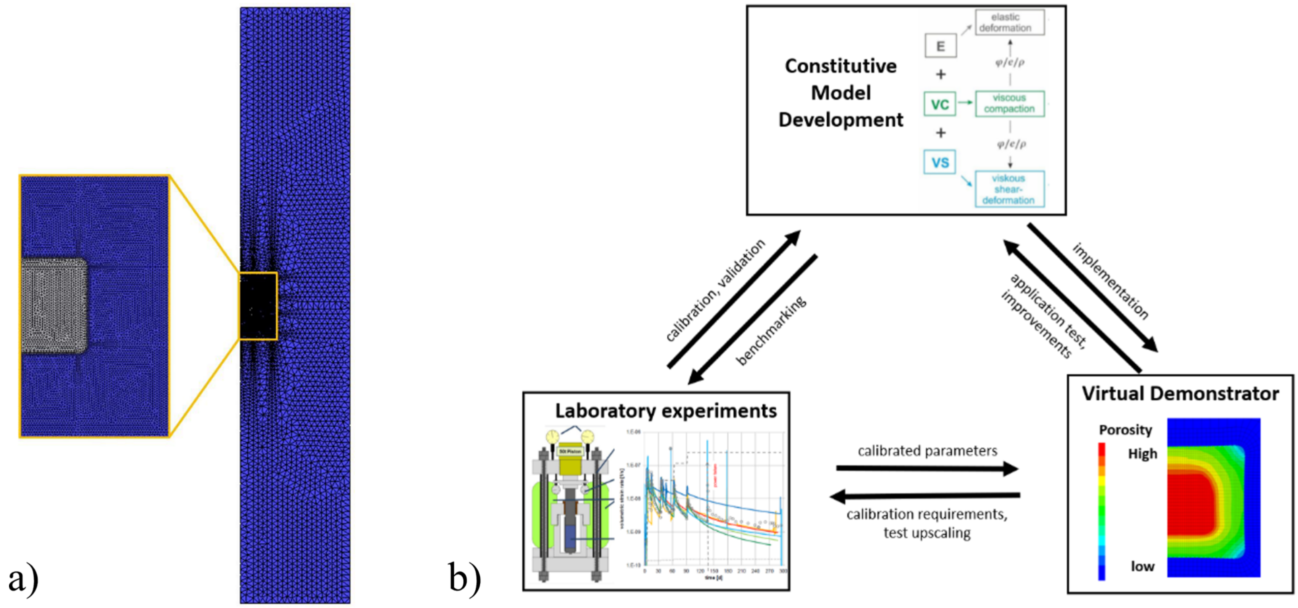

Figure 4. Virtual demonstrator. **(a)** Numerical model of a generic backfilled drift in rock salt. **(b)** Conceptual illustration of the role of the virtual demonstrator.

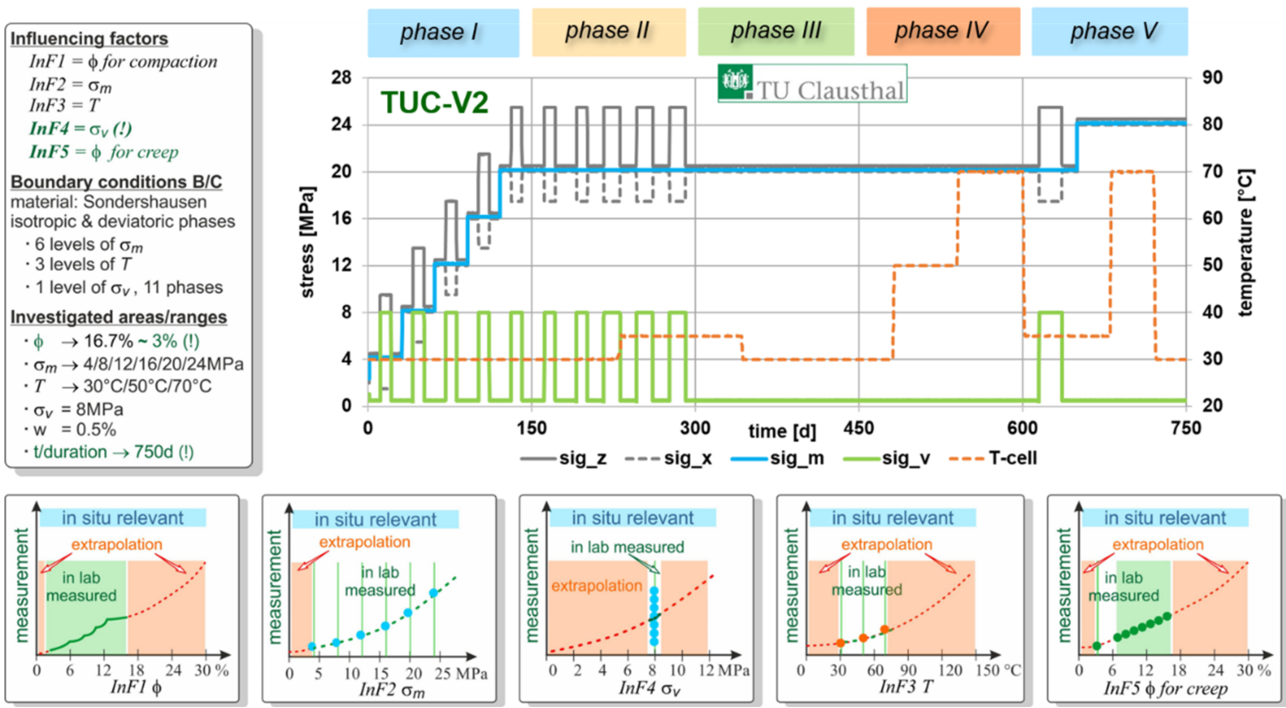

Figure 5. Thermomechanical loading program TUC-V2 applied in the long-term laboratory investigation of crushed salt compaction (Friedenberg et al., 2024).

tween laboratory-measured ranges and in situ-relevant conditions, highlighting the need for extrapolation for repository-scale applications. Initially, the TUC-V2 test was modeled with the limited knowledge available at the beginning of KOMPASS-I. Model development and optimization were performed to obtain a final model for the TUC-V2 test.

Figure 6 presents selected benchmark results for the TUC-V2 test after model development and/or optimization: the time-dependent evolution of volumetric strain (left panel)

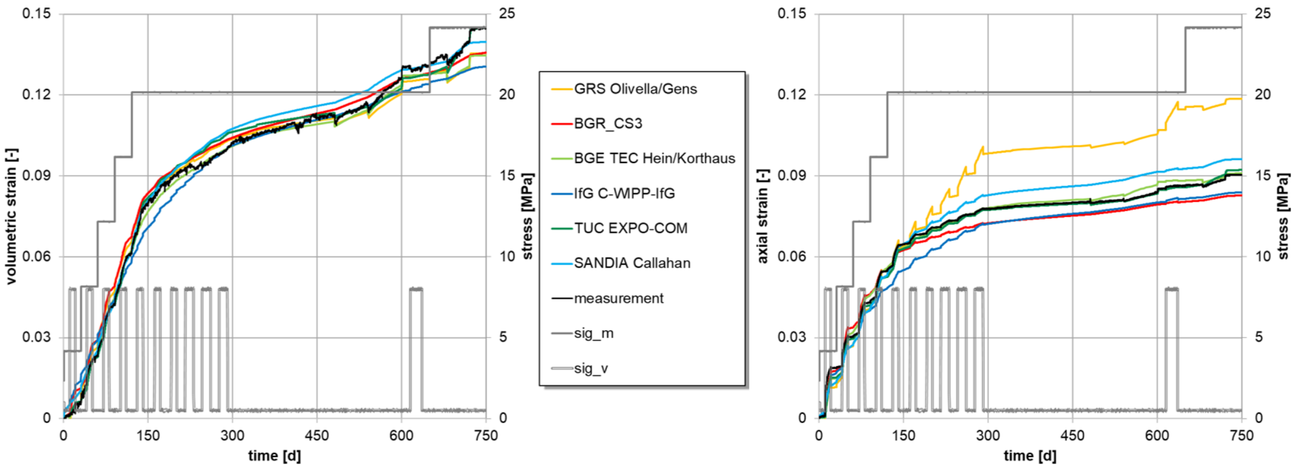

Figure 6. Benchmark results for the TUC-V2. Left: volumetric strain. Right: axial strain (Friedenberg et al., 2024).

and axial strain (right panel) for comparison across the different constitutive models. Experimental strain measurements are shown alongside the applied mean and deviatoric stress histories. The plot illustrates the characteristic rapid strain increase during the initial loading phase, followed by time-dependent creep deformation and continued strain accumulation under constant or stepwise mechanical loading over the 750 d test duration. Differences between model predictions highlight the variability in simulated compaction and axial creep behavior under identical thermomechanical boundary conditions.

Overall, the model results represent the best fits achievable with the currently available ("tostate") model formulations. For volumetric strain, the simulations show good agreement across modeling teams and with experimental data, indicating a consistent representation of bulk compaction processes. In contrast, a larger scatter is observed in the axial strain predictions. This variability can be attributed to differences in calibration priorities, where volumetric strain was generally emphasized over axial strain, as well as to known deficiencies in some constitutive formulations, such as an oversensitivity to changes in deviatoric loading. Additionally, variations in the representation of shear-induced creep mechanisms and stress redistribution contribute to the observed discrepancies. These results underline the need for further refinement of model formulations and calibration strategies to achieve a more balanced and robust reproduction of both volumetric and deviatoric creep behavior.

The virtual demonstrator is useful to indicate the continuous progress of numerical work. It is applied after each benchmark calculation, and porosity evolution is compared across the different models. Figure 7 compares the relationship between mean stress and porosity, averaged over the entire drift, for two successive evaluation stages. The left panel (status of KOMPASSI) illustrates the wide scatter in model predictions from different constitutive approaches in the absence of reference material data, leading to a large bandwidth in predicted porosity evolution with increasing mean stress. The right panel (KOMPASSII) shows the corresponding results after calibration against the TUC-V2 experimental database, demonstrating a clear reduction in the spread of model responses below 15 % porosity. Curves represent predictions from several numerical models, highlighting improved consistency in the stress–porosity relationship when experimental data are incorporated.

The demonstrator aided in identifying areas of focus for necessary calibration and model development. In the state of KOMPASS-I (left panel) the largest deviation in results is observed around 10 % porosity, determining the focus on the mid- to low-porosity level. In KOMPASS-II, the TUC-V2 triaxial compaction test covered a porosity range from 16 % to 3 % porosity, and by incorporating these data the spread in results is reduced for the mid- to low-porosity area (right panel). However, the results highlight the necessity of focusing on the high-porosity/low-stress regime, which is currently addressed within the MEASURES project.

Therefore, the arrows indicate the progressive reduction in result bandwidth, with further narrowing expected through the inclusion of additional datasets (TUCV4, TUCV5, and TK45). The comparison emphasizes the role of systematic experimental validation in adjusting constitutive model behavior for repository-relevant conditions. At the end of the MEASURES project, another run of the virtual demonstrator will be available. It is expected that bandwidth will be further reduced by incorporating more influencing factors and relationships.

5 Conclusion & outlook

The paper presents a systematic approach to improving the numerical predictive quality of crushed salt constitutive models in the context of a potential HLW repository in rock salt.

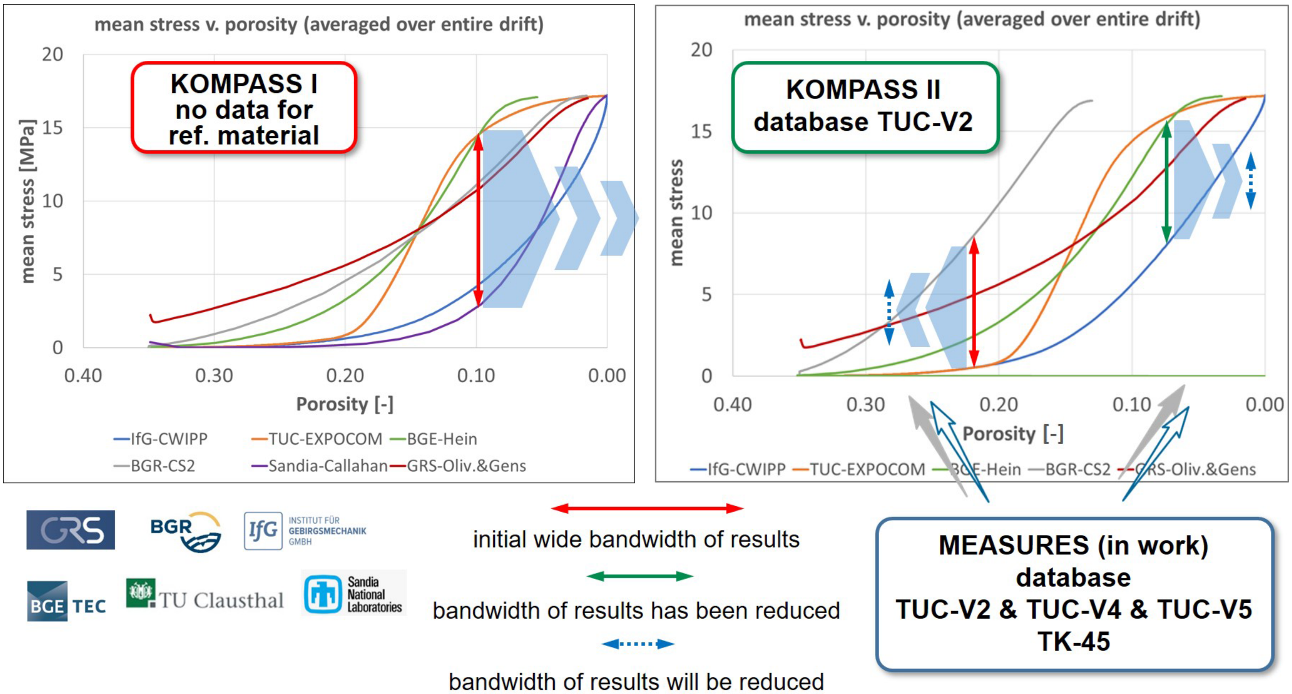

Figure 7. Results of the virtual demonstrator during the crushed salt projects.

The strategy focuses on a strong combination of experimental (compaction tests and microstructural studies) and numerical work, implemented iteratively. A continuously growing experimental database is initiated to systematically and independently investigate the main factors and processes influencing crushed salt compaction. By combining benchmark calculations, modeling, analysis, and development and/or optimization, a transparent approach to improving crushed salt constitutive models is established. The visualization of progress is ensured by the application of the virtual demonstrator.

The current status shows a successful application of the approach as the bandwidth of numerical results across different constitutive models has already been reduced through the incorporation of experimental data and the detailed investigation of influencing factors and processes. The work is not completed yet. Major achievements will be available at the end of the currently running MEASURES project (by the end of 2027).

Appendix A: Glossary

Wording	Definition
Confirmation	The process of assessing the correctness of constitutive model formulation from a qualitative perspective.
Constitutive model	Conceptual and/or mathematical description of the physical behavior of a particular material or substance.
Implementation	The process of translating a geomechanical model and its numerical solution strategy into executable computational algorithms within a specific software or code framework.
Modeling	The process of constructing an idealized representation of a geomechanical system – based on physics, constitutive theory, geometry, and assumptions – that describes how the system is believed to behave.
Prediction	Use of a model to foretell the state of a physical system under conditions for which the model has not been validated.
Simulation	The process of numerically solving the modeled problem to compute the system's response under prescribed conditions.
Uncertainty	A potential deficiency in any phase or activity of the modeling or experimentation process that is due to inherent variability (irreducible uncertainty) or lack of knowledge (reducible uncertainty).
Validation	The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.
Verification	The process of determining whether a model implementation accurately represents the developer's conceptual description of the model.

Code availability. The simulation codes used in this study are listed in Table 1. FLAC3D is a commercial software package provided by Itasca (2026, https://www.itascainternational.com/software/flac3d). JIFE is a proprietary in-house code developed and maintained by BGR and is not publicly available. Sierra/Solid Mechanics is a proprietary in-house code developed by Sandia National Laboratories and is not publicly available. CODE_BRIGHT is an open-source code provided by Olivella et al. (2026) (https://deca.upc.edu/en/projects/code_bright/downloads, last access: 5 August 2026).

Data availability. The datasets analyzed in this study are publicly available from their original source(s). As no dedicated data repository exists for these data, interested researchers should contact the corresponding author for details regarding data access and retrieval.

Team list. The MEASURES project family is an international composite of various organizations working together on the research into crushed salt compaction. The project family started to work together during the KOMPASS-I project (Czaikowski et al., 2020), followed up by the KOMPASS-II project (Friedenberg et al., 2024) and now proceeding into the MEASURES project (Friedenberg et al., 2025). The family members that are not listed as authors are presented as follows:

Jeroen Bartol (COVRA, the Netherlands), Hans De Bresser (Utrecht University, the Netherlands), Ann-Kathrin Gartzke (Federal Institute for Geosciences and Natural Resources (BGR), Germany), Suzanne Hangx (Utrecht University, the Netherlands), Kyra Jantschik (Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Germany), Matthew Kirby (Nuclear Waste Services (NWS), United Kingdom), Ben Laurich (Federal Institute for Geosciences and Natural Resources (BGR), Germany), Christian Lerch (BGE Technology GmbH, Germany), Lingyun Li (Institut für Gebirgsmechanik GmbH, Germany), Melissa M. Mills (Sandia National Laboratories, United States of America), Dirk Naumann (Institut für Gebirgsmechanik GmbH, Germany), Simon Norris (Nuclear Waste Services (NWS), United Kingdom), Bart Van Oosterhout (Utrecht University, the Netherlands), Benjamin Reedlunn (Sandia National Laboratories, United States of America), Nachinzorig Saruulbayar (Clausthal University of Technology, Germany), Christopher J. Spiers (Utrecht University, the Netherlands), Jan Thiedau (Federal Institute for Geosciences and Natural Resources (BGR), Germany), and Kornelia Zemke (Federal Institute for Geosciences and Natural Resources (BGR), Germany).

Author contributions. The whole MEASURES project family is responsible for the conceptualization of the projects, for the development of the research methodology, for conducting the research and the investigation process, and for providing all of the resources. LF wrote the paper draft. JK, SL, WL, and MR reviewed and edited the paper.

Competing interests. The contact author has declared that none of the authors has any competing interests.

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