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Discussions

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 to 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/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.

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Glossary

Wording	Definition
Confirmation	The process of assessing the correctness of constitutive model formulation from a qualitative perspective.
Constitutive model	Conceptual/mathematical description of a specific physical system.
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 that a model implementation accurately represents the developer's conceptual description of the model.

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 as 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 %).

The compaction process is determined by internal material properties (e.g., grain size/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. For predicting the evolution of crushed salt's sealing function in the safety analysis of a rock salt repository, understanding the complete compaction

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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 following primary achievements were:

- 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 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.
- Started to summarize a micro-physical process list combining literature research and own findings.
- Performing 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. Especially, 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.

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.

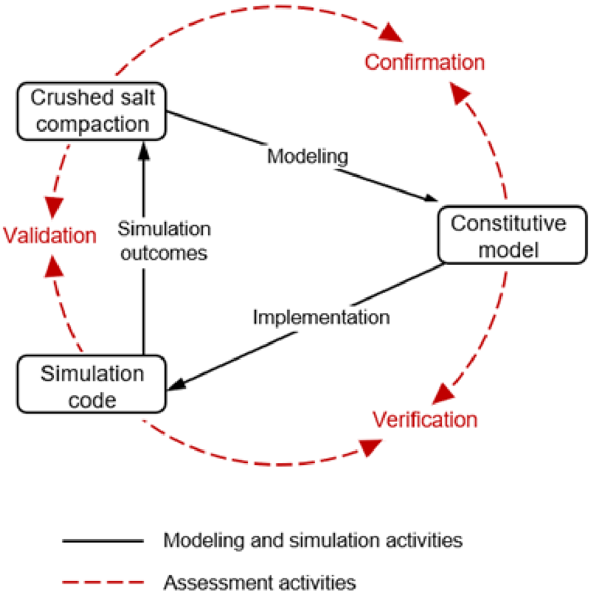

Figure 1: Schematic representation of the modeling, simulation, and assessment workflow for crushed salt compaction. Modified after Thacker et al. (2004).

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, aimed to be improved, supported by verification and validation activities. These contribute to 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 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.

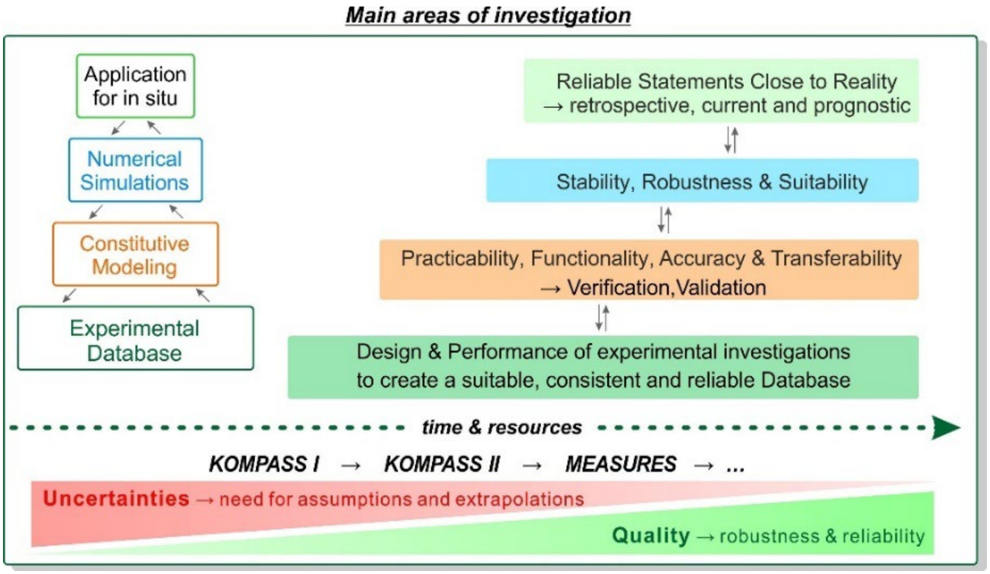

Figure 2: Overview of the main areas of investigation and methodological workflow for the development of reliable simulation-based statements.

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 (Figure 1) applies to laboratory tests and is planned to be expanded to in-situ applications in the future.

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 huge and not the focus of this paper. For more information, refer to the KOMPASS projects reports (Czaikowski et al., 2020; Friedenberg et al., 2024).

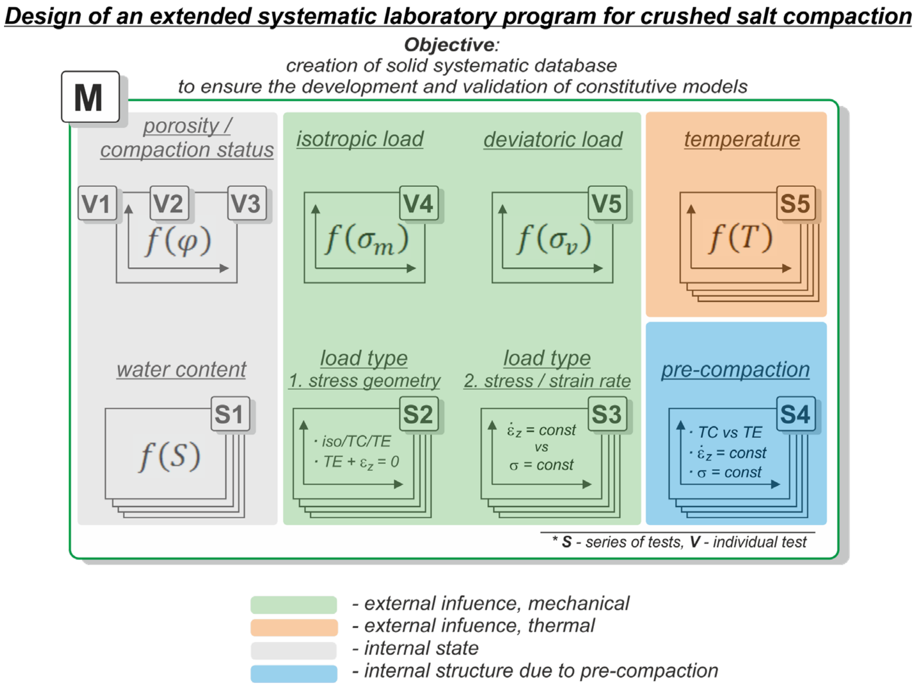

Figure 3: Systematic laboratory program as a basis for building the experimental database in the crushed salt projects.

A variety of constitutive models for crushed salt compaction are applied, as shown in Table 1. These models are 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/processes influencing compaction (especially moisture). Different constitutive models must be employed, and the results must be compared to building confidence, ensure quality assurance, and ensure robust results. Since there is no complete consensus on formulating constitutive models, uncertainties are avoided by using different formulation options to account for many complex physical processes and by using different methods (Finite Element Method/Finite Differences Method).

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

Organization	Constitutive model	Simulation Code	Method
BGE-TEC	Hein-Korthaus*	FLAC 3D	FDM
BGR	BGR-CS*	JIFE	FEM
GRS	CODE_BRIGHT model	CODE_BRIGHT	FEM
IfG	Modified C-WIPP model*	FLAC 3D	FDM
Sandia	Callahan model*	Sierra/Solid Mechanics	FEM
TUC	EXPO-COM**	FLAC 3D	FDM

*Models are under development/update

**Model is new developed in the frame of KOMPASS projects

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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 demonstrated using a virtual demonstrator representing a generic backfilled drift in rock salt (Figure 4a). Each time the investigation of a new factor/process is finished, the virtual demonstrator is applied, and the evolution of porosity (identified as the most important process variable) is evaluated. Using the virtual demonstrator ensures that all models capture the simplified behavior of rock salt in the same way, so that the only difference between the models lies in the constitutive model for crushed salt.

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

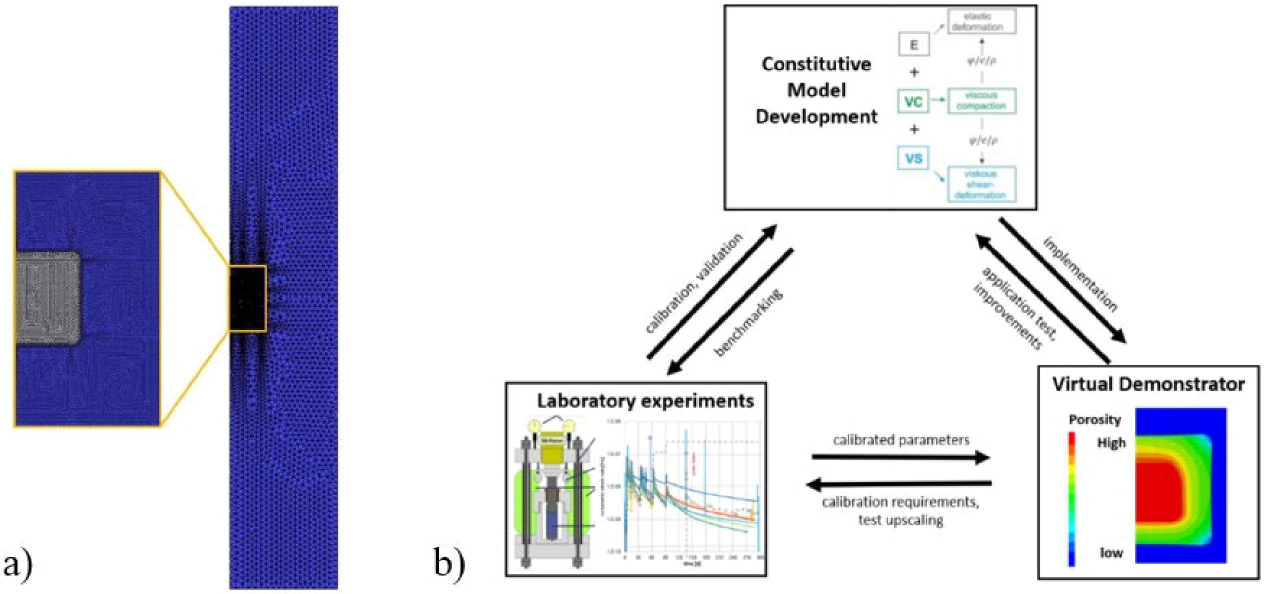

Figure 4: Virtual demonstrator. a) Numerical model of a generic backfilled drift in rock salt. b) Conceptual illustration of the role of the virtual demonstrator.

4 Application

The strategy presented above builds on an iterative approach of adding information, modeling, model development/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/optimization. Then, the virtual demonstrator is applied to the current state of the model and porosity evolution 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, so no data was 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 Figure 3), providing a solid basis for model development/optimization. The constitutive models are benchmarked against the triaxial compaction test TUC-V2, as shown in Figure 5.

The test is divided into five phases (I – V). The main plot shows the temporal evolution of stress components (σ_z = axial stress, σ_x = radial stress, σ_m = mean stress, σ_d = 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 days. 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 levels of deviatoric stress (σ_d), and three thermal levels. The left panel summarizes the influencing factors (InF) investigated in the study. These include porosity (Φ), mean stress (σ_m), temperature (T), and deviatoric stress (σ_d). 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 between laboratory-measured ranges and in-situ relevant conditions, highlighting the need for extrapolation for repository scale applications. Initially, the TUC-V2 test was modelled 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.

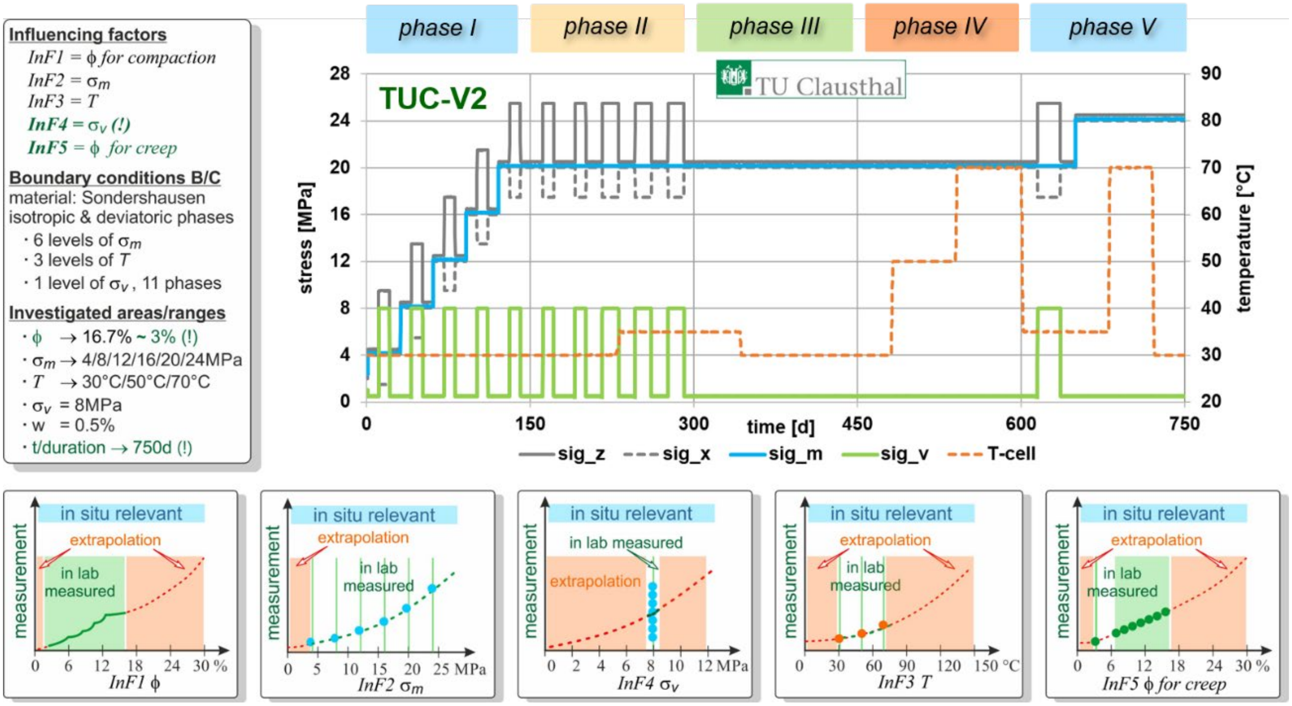

Figure 5: Thermomechanical loading program TUC-V2 applied in the long-term laboratory investigation of crushed salt compaction (Friedenberg et al., 2024)

Figure 6 presents selected benchmark results for the TUC-V2 test after model development/optimization: the time-dependent evolution of volumetric strain (left panel) 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-day test duration. Differences between model predictions highlight the variability in simulated compaction and axial creep behavior under identical thermomechanical boundary conditions.

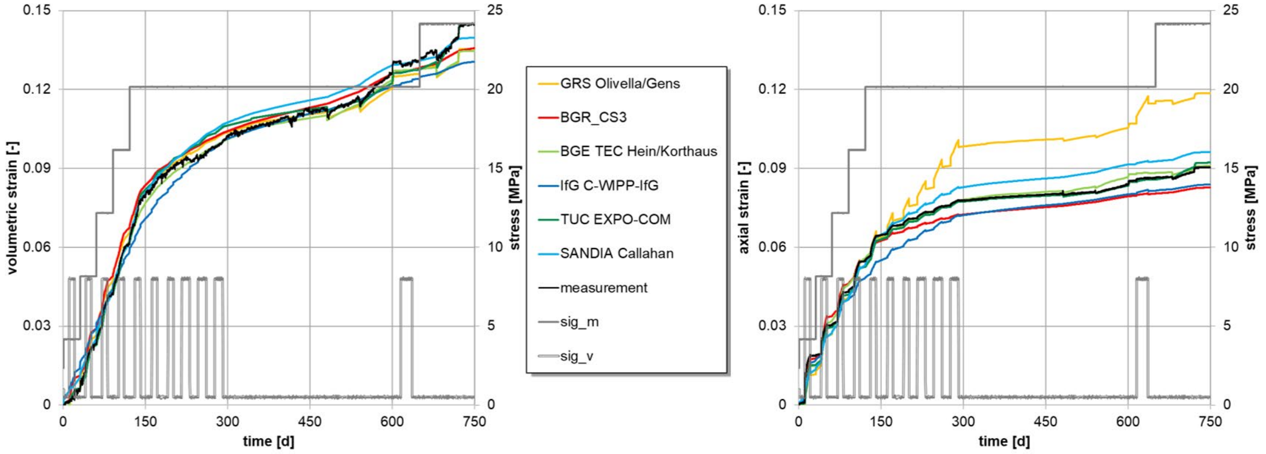

Figure 6: Benchmark results for the TUC-V2. Left: volumetric strain. Right: axial strain (Friedenberg et al., 2024).

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 KOMPASS-I) 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 (KOMPASS-II) shows the corresponding results after calibration against the TUC-V2 experimental database, demonstrating a clear reduction in the spread of model responses. Curves represent predictions from several numerical models, highlighting improved consistency in the stress–porosity relationship when experimental data are incorporated. The arrows indicate the progressive reduction of 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.

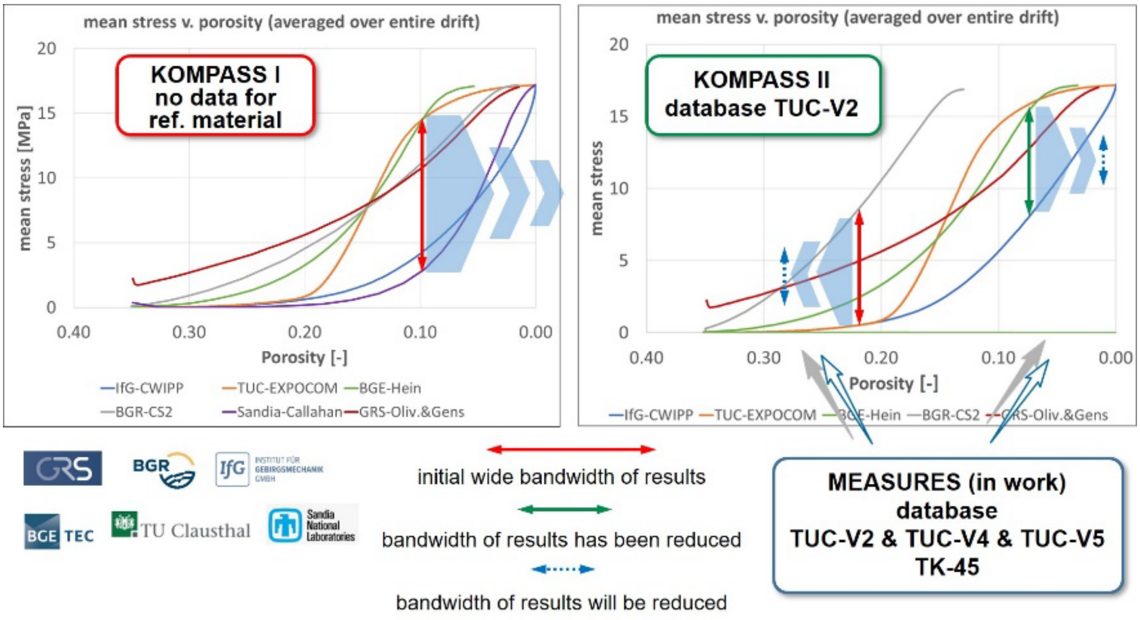

Figure 7: Results of the virtual demonstrator during the crushed salt projects

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. 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/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).

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Team list of the MEASURES project family members that are not explicitly listed as authors

The MEASURES project family is an international composite of various organizations working together in the research for crushed salt compaction. The project family started to work together in the KOMPASS-I project (Czaikowski et al. (2020)), followed-up by the KOMPASS-II project (Friedenberg et al. (2024)) and now proceeding in the MEASURES project (Friedenberg et al. (2025)). The family members that are not listed as authors are presented in the following Table 2:

Table 2: Members of the MEASURES project family that are not listed as authors

Last name, first name	Affiliation, Country
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Naumann, Dirk	Institut für Gebirgsmechanik GmbH, Germany
Norris, Simon	Nuclear Waste Services (NWS), United Kingdom
Van Oosterhout, Bart	Utrecht University, Netherlands
Reedlunn, Benjamin	Sandia National Laboratories, United States of America
Saruulbayar, Nachinzorig	Clausthal University of Technology, Germany
Spiers, Christopher J.	Utrecht University, Netherlands
Thiedau, Jan	Federal Institute for Geosciences and Natural Resources (BGR), Germany
Zemke, Kornelia	Federal Institute for Geosciences and Natural Resources (BGR), Germany

Author contribution

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 the resources; LF wrote the manuscript draft; JK, SL, WL, MR reviewed and edited the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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