

Design and Performance Assessment of Engineered Barrier Systems in a Salt Repository for HLW/SNF

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ABSTRACT: BGE TECHNOLOGY GmbH (BGE TEC) and Sandia National Laboratories (SNL) developed and jointly tested a methodology for the safety assessment of engineered barrier systems (EBS) for a high-level waste/spent nuclear fuel (HLW/SNF) repository in salt. Long-term isolation in such a repository is provided by a multi-barrier system including natural and engineered barriers. The salt provides the natural barrier, whereas the engineered barriers are different sealing components installed in the repository. The developed methodology is tested via a generic repository concept that is situated in a generic bedded salt formation. Based on this, a global model was generated, including relevant stratigraphic layers and underground openings of the repository. BGE TEC used this model to perform the integrity assessment of the shafts and drift sealings as main parts of the EBS. Simultaneously, SNL conducts the radiological performance assessment (PA). Both parts interact by an optimization of the EBS based on PA simulations and EBS-parameters. For this purpose, sensitivity analyses were incorporated into the PA simulation. This contribution presents the modeling and methodological approach used for BGE TEC and SNL for the design and performance assessment of EBS.

1 Introduction

RANGERS is an acronym for “Methodology for design and performance assessment of geotechnical barriers in a HLW repository in salt formations”. It is an ongoing joint project between BGE TECHNOLOGY GmbH (Germany), hereafter BGE TEC, and Sandia National Laboratories (US). It aims to develop a methodological approach to design EBS and how to handle them in the course of performance assessments in repositories in salt. The EBS design and construction methodology is based on the existing knowledge and experience of BGE, BGE TEC, Sandia, and others. The methodology will then be tested on a generic repository system in Germany. Four project sub-goals are formulated:

- Compilation of existing knowledge and experience in the design of geotechnical barriers and compilation of new concepts and technologies on the subject of geotechnical barriers.
- Development of a methodology based on the state of the art in science and technology for the design and verification of geotechnical barriers.
- Preliminary design and verification of the geotechnical barrier system for selected repository systems based on the developed methodology.
- Comparison of design results according to the new methodology with results of previous design and assessment.

The current priority roadmaps of the US Department of Energy Office of Nuclear Energy (DOE-NE) Spent Fuel and Waste Science and Technology (SFWST) campaign as well as of Federal Ministry for Economic Affairs and Energy of Germany highlight the value of international collaboration. BGE TEC and Sandia envisage therefore a deep collaboration in the project. The expertise of BGE TEC on modeling-based design of the EBS will be used to dimension the generic repository. The expertise of Sandia on performance assessment of large repository systems will be used to analyze the propagation of radionuclide through the engineered barrier systems and geochemical evolution of the generic repository design.

The current work summarizes the developed methodology for the design and verification of geotechnical barriers and describes the subsequent modeling concept necessary for the application of the proposed methodology. Finally, some numerical applications based on a generic bedded salt formation will be discussed.

2 Methodology

Based on international methodological standards, the evolution of HLW/SNF repositories in salt formations is analyzed in terms of a safety assessment, which means an assessment of the total system performance (IAEA, 2012), (NEA, 2014). Safety and the safety demonstration concept for salt repositories take full credit for the favorable properties of salt formations, including low permeability and porosity, high thermal conductivity, and self-healing behavior (Bollingerfehr et al., 2016), (Fischer-Appelt, 2013). The German repository concept is based on the safe containment of radioactive waste within the containment providing rock zone (CRZ), which requires the EBS (including the crushed salt backfill) to seal the perforation of the geological barrier by the mine excavations (BMU, 2020). The long-term safety of the mined excavations will be ensured by backfilling them with crushed salt. Crushed salt acquires its sealing capacity through compaction due to the convergence of the underground openings. Convergence is accelerated by waste heat and by humidity in the repository and water content in the host rock. Eventually crushed salt backfill will reach the same mechanical and hydraulic properties as the intact salt host rock. Until this time, the EBS ensures the waste isolation.

The present methodology summarizes all aspects of design and integrity assessment of the EBS, as well as their treatment in an eventual integrated performance assessment. Starting from the regulatory framework, a safety concept is defined. This is a basis for the development of repository and sealing concepts for the selected geological site. The evolution of the resulting repository system can be analyzed through preliminary analysis of the Features, Events, and Processes (FEP) catalogue, which includes all properties and possible evolutions that may occur in the repository system over the performance period.

While a comprehensive FEP analysis is not usually performed until after a site has been selected and characterized, the RANGERS methodology includes it, since there are aspects of EBS performance that can be studied by means of a focused preliminary FEP analysis using EBS-relevant FEPs. Ultimately, process models, based upon numerical models and experiments, are used to assess the integrity of the EBS as well as its impact in the integrated performance assessment simulations. For this purpose, the link between the (preliminary) FEPs and performance assessment is a key aspect of the proposed methodology. Based on the FEPs, the relevant loads (disturbances) affecting the EBS can be identified for the integrity assessment. The relevant processes have also to be modelled and considered in the

performance assessment. FEP interactions are described in scenarios. The relevant scenarios impacting the EBS and the repository can be derived from the FEP catalogue. A different procedure is provided for human intrusion impacts that are analyzed by stylized or “what if” type scenarios.

A reference scenario and two alternative scenarios were identified in the specific FEP analysis carried out for RANGERS. The reference scenario implies the EBS (i.e., shaft and drift seals) retains its function over 50,000 years, what is considered up to the next ice age in Germany (Müller-Hoeppe et al., 2012). It is expected that the hydro-geologic and topographic conditions will change significantly at the next ice age, so that an accurate prediction of the geochemical composition of the inflowing waters becomes impossible. The first alternative scenario involves the shaft seal losing its function but drift seals retaining their function. In the second alternative scenario, the opposite is assumed: the drift seals lose their function and the confinement of the emplaced waste relies solely on the shaft sealing system. For each of these scenarios, three different cases for fluid migration are assumed:

- Case 1: Water flows from overburden through the shaft seal to the disposal zones
- Case 2: Gas migration inside the repository from corrosion of the casks
- Case 3: Water source inside the repository from inter-/ intragranular salt solutions

At this stage, numerical modeling is being performed to assess the integrity of the EBS and its impact on the integrated performance assessment (PA) simulations. For this purpose, the link between the two kinds of assessment is a key aspect of the proposed methodology. The main idea is to increase the physical realism of the repository PA simulations by comprehensive and specific analyses of the behavior of the EBS under thermal-hydrological-mechanical and chemical (THMC) conditions. The results of these analyses can be considered in the PA modeling, thus increasing realism and reducing the material and model uncertainties describing the EBS in the PA model. Figure 1 gives an overview of the proposed methodology.

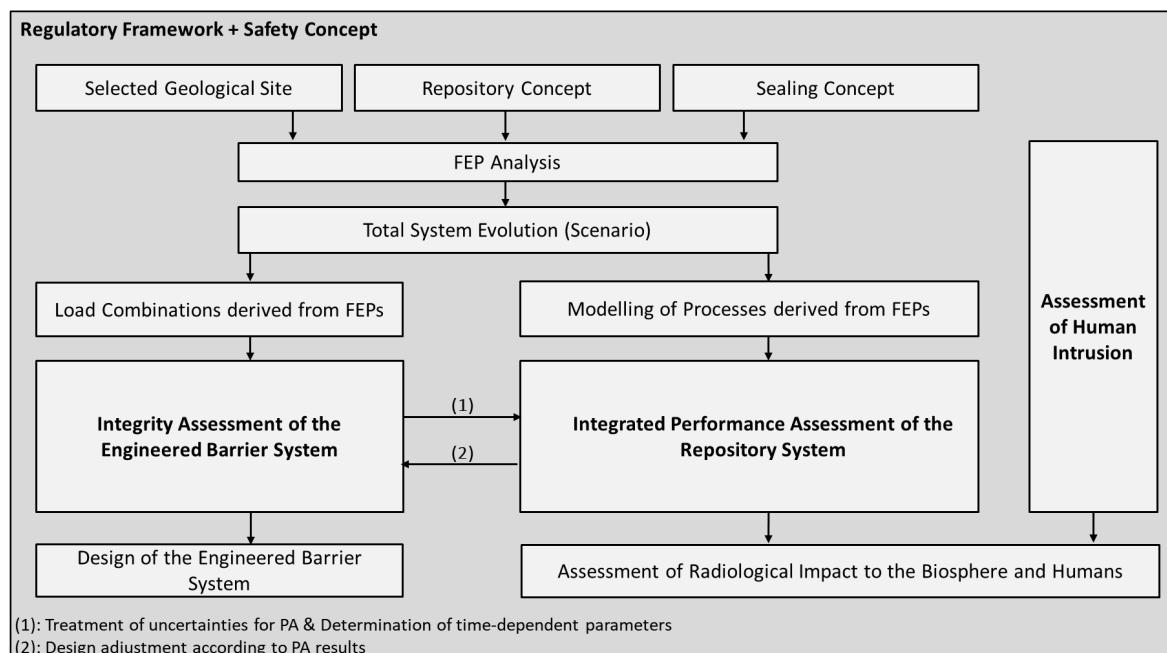


Figure 1: Methodology for the design and performance assessment of the EBS in a salt repository.

3 Modeling and Verification Concept

3.1 Integrity assessment of the Engineered Barrier System

Because the EBS is an engineered structure, the procedure for EBS performance assessment can rely on adequate regulations or recommendations. In Germany, the EBS is seen as a set of civil engineering structures, and their adequate design has to be verified by a technical proof in accordance with EUROCODE and respectively with its national implementations DIN EN 1997-1 and DIN EN 1990, (Müller-Hoeppel et al. 2012). The EUROCODE is a semi-probabilistic, reliability-oriented safety assessment concept using partial factors. In the USA, the Building Code Requirements for Structural Concrete (ACI 318-14) can be considered for the design of the EBS in compliance with other local regulations. The aim is to verify the required level of reliability of EBS construction by verifying that the loads acting on the structure do not exceed the inherent strength or resistance of the structure. For the specific integrity assessment of the EBS, the demonstration of sufficient hydraulic resistance (demonstration of tightness) and the demonstration of the sufficient load bearing capacity (structural integrity) must be verified individually. Additionally, assessment of constructability must be included, due to the uniqueness of EBS as structure. For the demonstration of the tightness, the contact zone between seal and surrounding rock, as well as the excavation-damaged zone in the surrounding rock, must be considered in addition to the constructed barrier itself. Demonstration of structural integrity requires individual assessment of structural stability, crack limitation, and deformation limitation. For soil-based components, the filter stability must also be verified. The functional lifetime of the EBS significantly exceeds the usual functional lifetime of conventional civil engineering structures (50 to 100 y). To ensure applicability of the EUROCODE over the functional time of 50,000 years, a long-term stability criterion is introduced. This criterion assesses how the materials and components of the EBS may deteriorate over time in each material. Example phenomena affecting the long-term performance of the EBS materials include creep and shrinking in concrete, the geochemical evolution of the repository system or the effect of temperature. The overall verification concept for the EBS is summarized in Figure 2.

Due to the complexity of the processes taking place within the repository system, the determination of mechanical, thermal, hydraulic or chemical loads acting on the repository can only be carried out through numerical modeling. To verify the assessment criteria mentioned above, a methodological modeling approach has been developed within project RANGERS. In this regard, each possible scenario evolution case derived from the specific FEPs is considered a verification case. Based on the understanding of the processes considered in the scenarios, one determines the processes necessary to assess each of the criterion of the verification concept. For instance, the assessment of the hydraulic resistance of the EBS can obviously be derived by analyzing the hydraulic evolution of the repository system. The hydraulic resistance is verified when the resulting flow rate within the EBS stays below the limit set in the German repository safety concept (in the US, regulations do not apply to individual system components). Processes can be combined if concurrent processes may affect the criterion under consideration. This is for example the case when compaction of crushed salt leads to a decrease of permeability in the system. In this case, the effect of the compaction in the assessment of the hydraulic resistance can be considered explicitly through coupled hydro-mechanical analyses or implicitly through the consideration of permeability and porosity due

to compaction in the hydraulic analyses. The swelling behavior of bentonite can be considered similarly. Several individual assessments can be carried out simultaneously in the process modeling, once the material properties have been evaluated. This is for instance the case for the sealing element, the element-host rock contact zone, and EDZ, which are usually part of a single numerical model. When the material constitutive models allow, individual structural integrity assessments can also be combined. Following these reflections for each considered scenario, a simulation matrix can be constructed, connecting the scenarios (or the FEPs) with the assessment criteria coming from the verification concept (or the building codes). Such a matrix is presented in Figure 3 for the generic repository system analyzed within RANGERS.

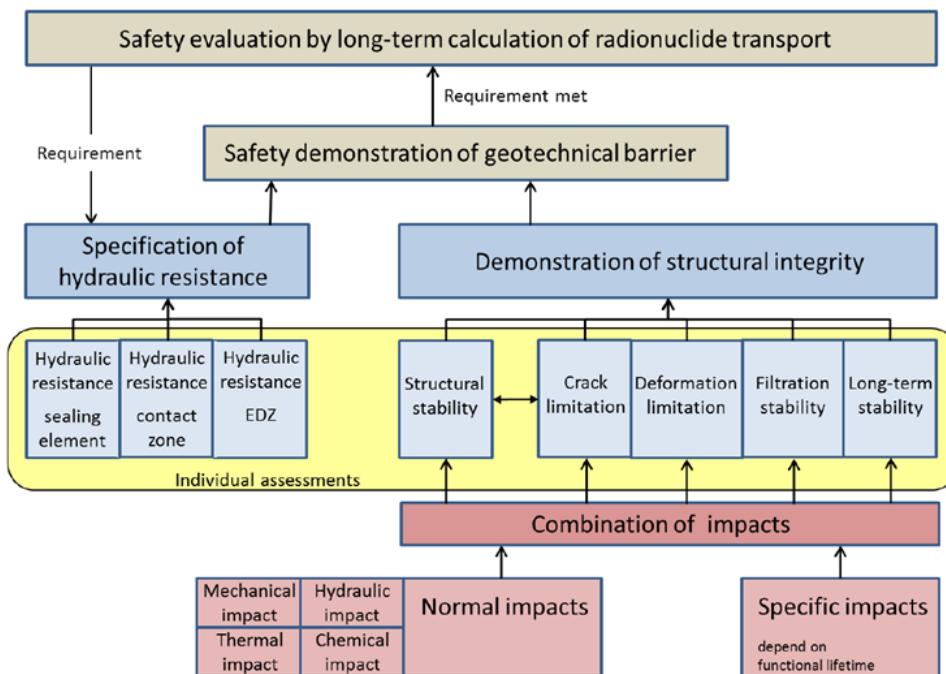


Figure 2: Verification concept for the integrity assessment of EBS based on German Regulatory Requirements (Müller-Hoeppel et al., 2012).

| Specification of hydraulic resistance | | | Demonstration of structural integrity | | | | |
|---|--|---|---------------------------------------|--|------------------------|----------------------|---------------------|
| Hydraulic resistance -sealing element | Hydraulic resistance -contact zone | Hydraulic resistance -EDZ | Structural stability | Crack limitation | Deformation limitation | Filtration stability | Long-term stability |
| Reference Scenario: The EBS retains its function over 50000 years | | | | | | | |
| Case 1: Water flow from overburden through the shaft to the disposal zones | H: determination of flow rate and passing time (constant permeability) HM: including compaction of crushed salt (time dependent permeability) | TM: structural analysis of the EBS components | No modelling intended | C: determination of geochemical stability of the sealing elements against water/brine T: temperature effects on EBS-materials | | | |
| Case 2: Gas production inside the repository from corrosion of the casks | HM: crushed salt compaction under gas pressure build up | No modelling intended | No modelling intended | No modelling intended | | | |
| Case 3: Water source inside the repository from inter- / intragranular salt solutions | H: determination of flow rate and passing time (constant permeability) HM: including compaction of crushed salt (time dependent permeability) | TM: structural analysis of components inside the drift (concrete abutments) | No modelling intended | Geochemical analysis: determination of geochemical stability | | | |

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Figure 3: Modeling matrix for the integrity assessment of the EBS.

3.2 Integrated repository system performance assessment

To carry out PA simulations of the repository, the identified scenarios must be broken down into process groups affecting the components of the EBS and the geological barrier. Examples of processes derived from the scenarios include: advection and diffusion phenomena (linked to alteration of the EBS and to radionuclide transport), compaction of crushed salt, creep of salt, and heat propagation in the repository. The impacts of considering such processes in the PA must carefully be considered. Because of the large model domain, long time scales, and the need for uncertainty quantification in PA simulations, not all processes can be explicitly included. Sometimes separate process models must be used to understand the evolution and importance of key parameters over time, and how these effects can be best presented in PA. The current approach for Geologic Disposal Safety Assessment (GDSA) Framework in the US (LaForce et al., 2020) builds upon previous salt reference cases (Sevougian et al., 2016) for deep geologic disposal of defense-related HLW and SNF. Subsequent developments to the GDSA framework make it now possible to assess most of the relevant processes in a single numerical model (LaForce et al., 2020; 2021; Nole et al., 2021). Processes accounted for in the conceptual model include waste package degradation, waste form (UO_2) dissolution, equilibrium-controlled radionuclide sorption and precipitation/ dissolution, radioactive decay and ingrowth in all phases (aqueous, adsorbed, precipitate), coupled heat and fluid flow, and radionuclide transport via advection and diffusion. Implicit mechanical effects are not yet considered in GDSA PA simulator, but are part of process modeling (TOUGH-FLAC). Due to the massively parallel nature of PFLOTRAN (Hammond et al., 2014) it is possible to represent the repository system with a high level of geometric and configurational complexity. The conceptual framework for the salt reference case focuses on the components of the engineered barrier and the natural barrier and assumes an undisturbed scenario outside the repository zone. In the same way alternative scenarios can be assessed.

Building on this background, the RANGERS project is deriving all relevant processes from the FEPs and scenario evolution that should be considered in the process modeling. Similar to the integrity assessment of the EBS, the different scenario evolution cases are assumed separately as verification cases. Here, concurring scenario evolution cases can be combined, depending on the capabilities of the simulator used. In PFLOTRAN, water and gas flow within the repository can explicitly consider the effects of gas production in the repository. For each analyzed verification case or combined cases, the target criteria assumed for the PA must be verified. Following the German regulations (BMU, 2020, para 4), the safe containment of radionuclides in a repository should be demonstrated by assessing the mass of radionuclides discharged through the essential barriers. The mass fraction of radionuclides leaving the CRZ must stay below 10^{-4} cumulatively and 10^{-9} annually for the verification period. For spent fuel and high-level waste in the US, rather than a simple mass fraction, most recent regulations stipulate a maximum annual dose (15 mrem/yr before 10,000 years and 100 mrem/yr after) to a hypothetical exposed future individual (DOE, 2008). Additionally, a groundwater protection standard is included to protect drinking water. In Germany, exposures due to discharges of radionuclides are negligible if the estimated additional effective dose for individuals of the population is at most in the range of 10 mSv (1,000 mrem) per calendar year, and for the deviating evolutions, the estimated additional effective dose for individuals of the population does not exceed 100 mSv per calendar year (BMU, 2020, para 7).

4 Numerical Applications

To test the developed methodology, a generic repository system is considered. The selected generic geological formation is a salt pillow formation developed within the project KOSINA (Bollingerfehr et al., 2018). Within this formation, a repository has been located where the salt formation is thickest. The repository planning assumes a maximum temperature of 200 °C at the surface of the waste casks. To meet this temperature requirement, the repository has been thermally designed to optimize the spacings between the drifts and between the disposal casks within the drifts. The resulting repository system is represented in Figure 4. The engineered barrier systems of this repository consists of four horizontal closure systems installed in the main drifts near sealing the two emplacement wings and of two shaft closure systems installed in both shafts. Each of these horizontal closures is 500 m long and is divided into two abutments made of magnesia (i.e., Sorel) concrete with a length of 50 m. In between the abutments, the 400 m long backfill seal is made of a mixture of crushed salt and clay, which itself seals after reconsolidation and compaction, taking over the long-term sealing function of the repository. For up to 50,000 years, the concrete abutments should limit any potential fluid migration within the repository mine and should protect the crushed salt seal against hydromechanical loads. The shaft closure system is made of several material following the concept of diversity and redundancy. The shaft closure is redundant to the drift closure. The sealing elements made of Sorel concrete, salt clay, and bentonite ensure the diversity and the redundancy of the closure system. If one seal loses its function, other seals made of different material will significantly reduce the chance that the same deficiency occurs in multiple elements.

Two simulation cases will be discussed in the following to illustrate the proposed methodology.

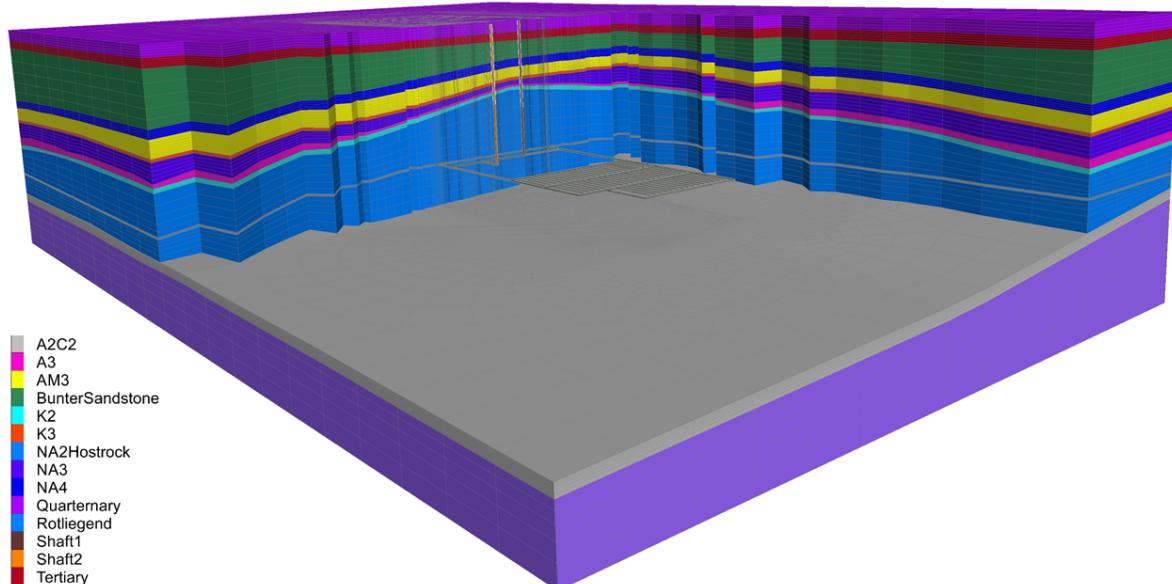


Figure 4: Generic repository system of a salt pillow formation used in RANGERS.

4.1 Verification of the long-term stability of EBS-components based on thermal simulation

High temperature can affect the long-term performance of the EBS materials. As part of the assessment of the long-term stability criterion, the temperature evolution in the repository is evaluated, see Figure 3. The numerical model for this assessment includes a detailed representation of the whole repository system with dimensions of several km on each side. The thermal load has been homogenized in each drift based on the heat power of the radioactive waste disposed in the drift. A more detailed analysis at the level of drift where each component within the drift is discretized have been performed during the thermal design of the repository. Due to the homogenization and reduction in the ability to represent steep temperature gradients between the cask and surrounding material, the maximum temperature in the homogenized drift is about 130°C compared to 200°C at the surface of the cask when individual disposal casks are represented in the numerical model. Nevertheless, this discrepancy only occurs in the nearfield and the developed numerical model is believed to be precise enough for the temperature evolution in the far field. Figure 5 shows the thermal evolution of the system after 500 years, by which time the repository mine has reached its maximum. In the figure, one can see how the heat propagates through the geological formation. This propagation is asymmetric between the two emplacement fields due to the different heat power of the different families of radioactive waste emplaced in the repository

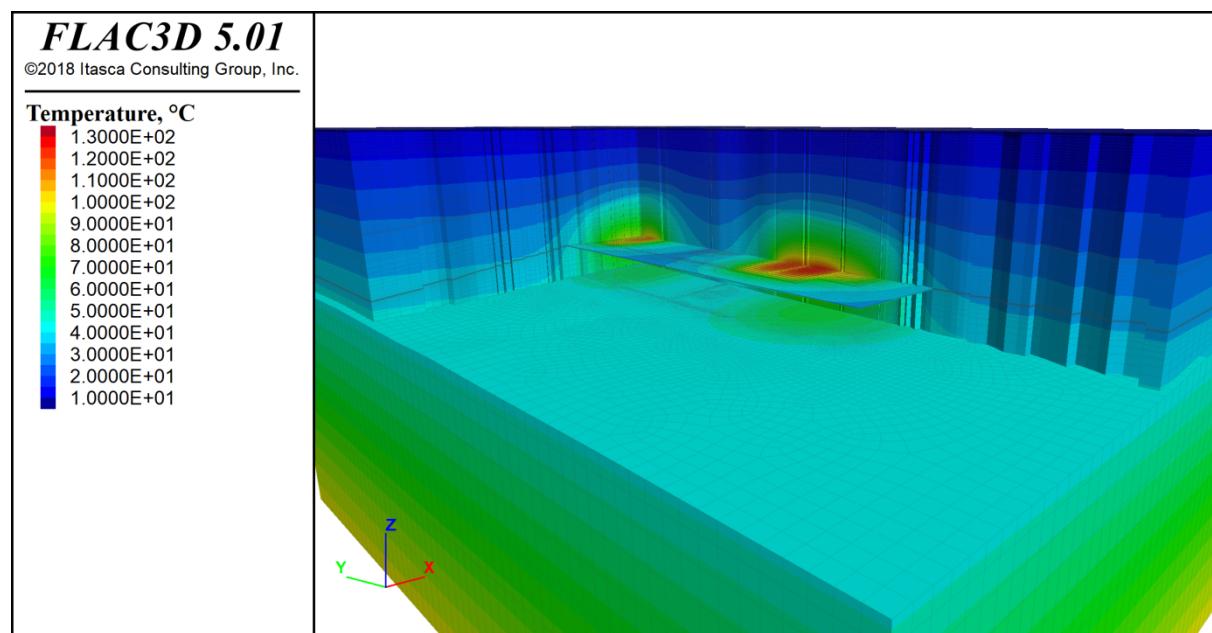


Figure 5: Thermal evolution in the repository system at 500 years.

The evaluation of the temperature evolution in the engineered barriers is shown in Figure 6. In the first 1,000 years the maximum temperature increase in the shaft is about 5 °C. In the drift seal a maximum temperature increase of 20 °C occurs around 400 years. The drift seal starts subsequently to cool down reaching a temperature increase of less than 15 °C after 1200 years near the emplacement field. In regard to the long-term stability of the EBS components, one can conclude that due to the negligible temperature increase in the EBS, the temperature evolution will not endanger the long-term stability of the geomaterials used in the EBS. For instance, the sealing properties of clays and bentonite do not deteriorate when exposed to temperature up to 100 °C (Villar et al., 2020). Rock salt from bedded salt formation in Germany with a water content of 0.02 up to 2% - only shows disintegration ("decrepitation") linked to the

formation of microcracks above approx. 250 °C, (Bräuer et al., 2016). Sorel and salt concretes are stable up to 90 °C. This temperature limit increases with the *in situ* confining pressure that is to be expected in repository conditions. Higher confining stress will reduce the development of fractures.

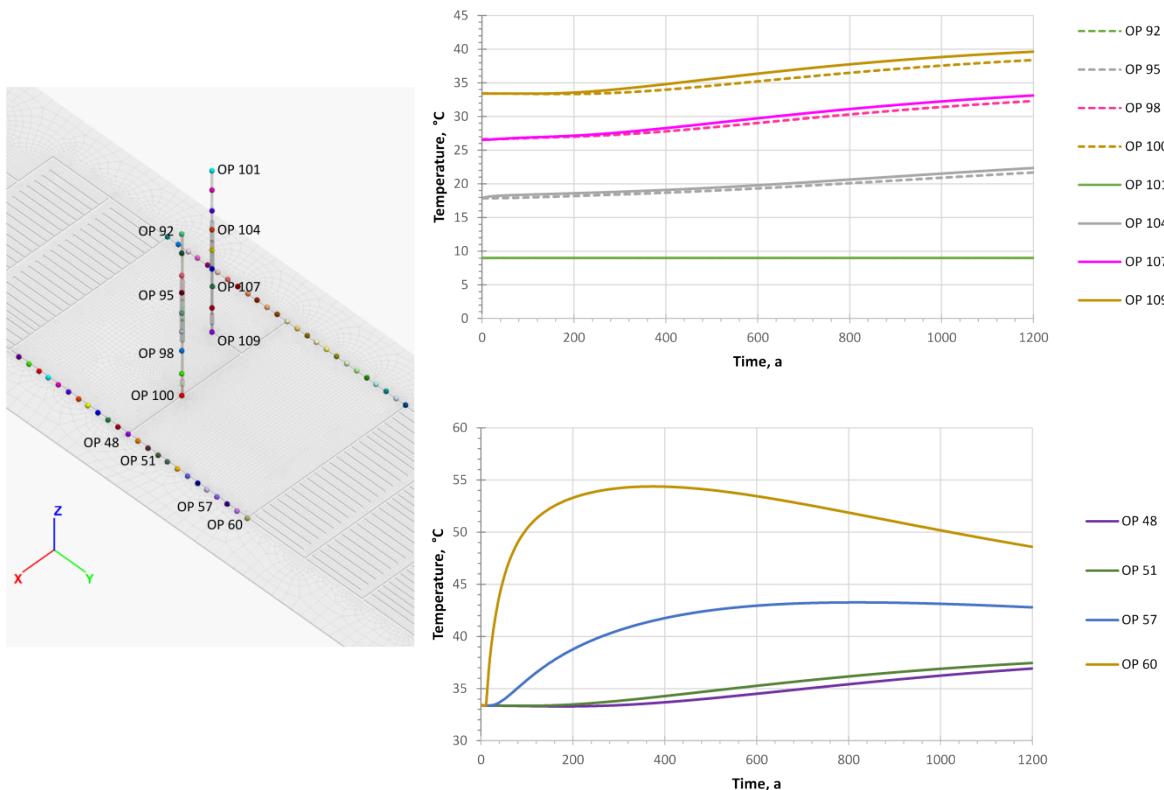


Figure 6: Evolution of the temperature in the shaft and drift closure systems.

4.2 Preliminary long-term evolution of the repository system for the reference scenario case

For a realistic PA, a coupling between the integrity assessment and the integrated performance assessment has been proposed in the methodology, see Figure 1. The coupling consists of determining the time dependent hydraulic behavior of the EBS components upon thermomechanical loads that occur due to the compaction of the salt host rock. These time-dependent parameters will then be used to describe the hydraulic behavior of the EBS in the scope of the performance assessment. This approach is useful as mechanical processes are challenging to efficiently include in the PA due the long timescale of such simulations, and the typical requirement of uncertainty quantification through Monte Carlo, requiring numerous model runs.

In this context, thermal-mechanical analyses of the compaction of the crushed salt backfilled in the working mines of the repository have been realized. The simulations are based on the same numerical model shown in Figure 4 as well as on the thermal analyses in Figure 4 into incorporation of mechanical effects. The behavior of crushed salt is described by a visco-plastic model (Bertrams et al., 2020). The BGRa model is used to describe the creep behavior of rock salt (Bertrams et al., 2020). The resulting compaction of crushed salt (i.e., change in porosity from initial value of 0.35) at 100 years is depicted in Figure 7. The porosity distribution is a function of the thermal evolution at each location. Generally, the higher temperature correlates

with higher compaction, with the exception made for “cold” drifts surrounded by “hot” drifts. With the determined porosity, the permeability in the repository can be determined. Both data will be subsequently used in performance assessment simulations.

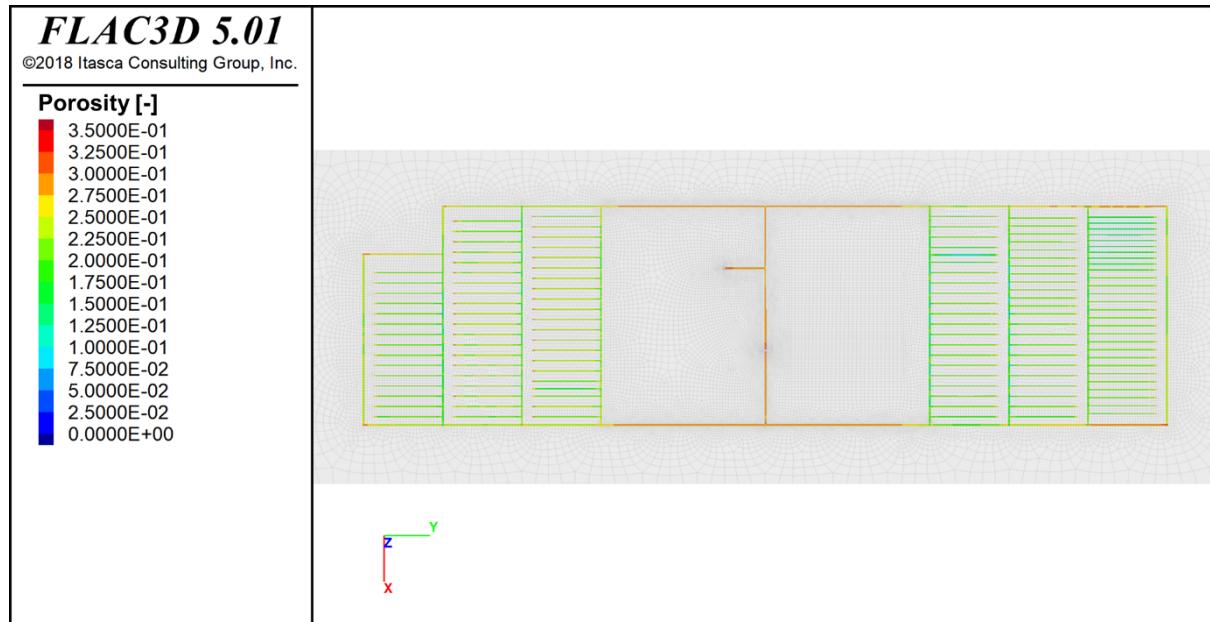


Figure 7: Porosity distribution in the drift system backfilled with crushed salt at 100 years

The results of the thermal-mechanical simulation, giving porosity through time will be included as inputs to PFLOTRAN, which will compute the thermal-hydrological response of a system on the same solution mesh, with the same thermal sources, and the specified porosity from the results of the thermal-mechanical model. Decreases in porosity lead to increases in both gas and liquid pressure, and since gas is more compressible than liquid, the liquid saturation tends to increase.

5 Conclusion

Within the framework of the project RANGERS a methodology for the generic design and performance assessment of EBS in a repository in salt has been developed. The methodology consists of a workflow to assess the integrity of engineered barrier systems in repositories in salt. The consideration of the EBS in the scope of integrated performance assessments is also part of the proposed methodology. To apply the methodology, a modeling and verification concept is proposed. The methodology is currently being applied on a generic repository system in a bedded salt formation. Based on this, a global model was developed to carry out different numerical assessments that have been derived from the application of the modeling concept. Two of these assessments have been presented in this work. Further assessments will be carried out in the next phase of the project to completely design the EBS according to the regulations in force. The role of the EBS and the uncertainties concerning their treatment in the scope of performance assessment will be also investigated.

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