Long-term safety analysis and model validation through URL research

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Abstract: In Germany, all types of radioactive wastes will be disposed of in deep geological repositories. While a repository for low-level radioactive waste (LLW) has recently been licensed, different host rock formations are considered for disposal of heat producing high-level waste (HLW). The latter includes directly disposed spent fuel (SF) and vitrified waste from its reprocessing. Different canisters and disposal concepts are considered for spent fuel disposal, i.e. thick-walled iron casks in horizontal drifts or thin-walled BSK3 steel casks in vertical boreholes.

GRS is the leading expert institution in Germany concerning nuclear safety and waste management. For the recent 30 years, GRS has developed and continuously improves a set of computer codes, which allow assessing the performance and the long-term safety of repositories in various host rocks (salt, clay or granite) adopting different technical options. Advanced methods for deterministic as well as probabilistic assessments are available. To characterize the host rocks and backfill/buffer materials and to develop disposal technologies, comprehensive laboratory experiments and a large number of in-situ tests have been performed at GRS’ geo-laboratory and underground research laboratories in different host formations. Thermo-hydro-mechanico-chemical (THMC) processes occurring in the host rocks and engineered barrier systems are numerically simulated.

The paper presents an overview of GRS’ work highlighting important results of performance assessment (PA) studies for both the salt and clay options. Also, recent results of in-situ investigations and laboratory studies are presented together with modeling results. Special emphasis is dedicated to the consideration of coupled THM processes which are of relevance in PA.

Key words: high-level radioactive waste; disposal; clay; salt; buffer; performance assessment (PA)

1 Introduction

GRS is the leading expert institution of Germany in the field of nuclear safety in general. The division at Braunschweig mainly researches on final disposal of radioactive waste, either in-situ or in the laboratory. Theoretical and experimental investigations are performed on the process level as well as on the integrated level. A great variety of computational tools for these investigations are available, some of these are developed by GRS itself.

The experience of GRS is used by implementers in the development of safety cases for repository projects. Thus, GRS has contributed to all repository projects in Germany, especially to safety analyses.

To prove existing models and to improve the tools, investigations on the process level are performed. This includes work in underground research laboratories, where GRS is involved in projects in several countries.

2 Experience of GRS

Throughout the past 30 years, GRS staff has gained experience in all topics related to radioactive waste disposal, e.g. in-situ disposal techniques, modeling of processes relevant for radioactive waste disposal, code development, long-term safety analyses. Table 1 lists some of the most relevant current projects. During the last decade, the computer codes d3f and r1t have been developed, which allow 3D calculations of groundwater flow and transport of contaminants in large and hydro-geologically complex areas taking into account, among others, density effects and chemical retardation during transport. Several national projects are dealing with the preparation of a safety case for a high-level radioactive waste (HLW) repository in salt formations. The tools for safety analyses in clay formations have been developed recently. Currently, GRS is involved in the safety analyses for closing the low-level radioactive waste (LLW) repositories at Morsleben (ERAM) and Asse sites.
Table 1 Current projects.

<table>
<thead>
<tr>
<th>Type of work</th>
<th>Project</th>
<th>Formation</th>
<th>Type</th>
<th>Objective</th>
<th>Period</th>
</tr>
</thead>
<tbody>
<tr>
<td>Research and development</td>
<td>r3t, d3f</td>
<td>Porous</td>
<td>National</td>
<td>3D transport simulation</td>
<td>Until 2004</td>
</tr>
<tr>
<td></td>
<td>ISIBEL</td>
<td>Salt</td>
<td>National</td>
<td>Pre-project for the safety case of a repository for HLW</td>
<td>2007–2010</td>
</tr>
<tr>
<td></td>
<td>REPOPERM</td>
<td>Salt</td>
<td>National</td>
<td>Remaining backfill porosity in the long term</td>
<td>2008–2012</td>
</tr>
<tr>
<td></td>
<td>FUNMIG</td>
<td>Clay</td>
<td>International</td>
<td>Radionuclide migration</td>
<td>2003–2007</td>
</tr>
<tr>
<td></td>
<td>PAMINA</td>
<td>Various</td>
<td>International</td>
<td>State of the art in PA</td>
<td>2006–2009</td>
</tr>
<tr>
<td>Safety analyses</td>
<td>ERAM</td>
<td>Salt</td>
<td>National</td>
<td>Safety proof</td>
<td>Since 1996</td>
</tr>
<tr>
<td></td>
<td>Asse</td>
<td>Salt</td>
<td>National</td>
<td>Safety proof</td>
<td>Since 2002</td>
</tr>
</tbody>
</table>

3 Integrated computer codes

To assess performance and long-term safety of a repository, integrated computer codes are used, which comprise models for all relevant effects of the system. It is common practice to divide a repository system into the following compartments: near-field, far-field and biosphere, and to use individual codes (modules) for each of these compartments. Figure 1 presents the available modules of the computer code package EMOS [1]. These modules are applied to the calculations presented below.

![Fig.1 Available modules of EMOS package.](image)

The modules for each compartment include numerical models for module-specific transport processes. Figure 2 gives an overview of the most relevant processes considered. While radioactive decay, temperature evolution, etc. (upper part of Fig.2) are taken into account in all modules, diffusion and sorption are considered in far-field modules; while in near-field modules, advection, dispersion, diffusion, and convection are considered as transport processes besides other effects.

The models of the integrated computer codes are supported by investigations with process level codes, as described later.

The integrated codes of GRS have been applied to several international projects and benchmark exercises [2–4]. These exercises demonstrated the high quality of the PA tools.

4 Application of integrated computer codes

4.1 Modeling of repository systems

The integrated computer codes of GRS are available for different kinds of repository systems, including different host rock formations, i.e. salt, clay or hard rock formations. These codes were applied to various disposal projects in Germany, including the existing LLW repository ERAM [5], the former research mine Asse [6], and the scheduled LLW repository Konrad [7]. As there is no decision about HLW repositories in Germany up to now, the application of the codes to HLW repositories is only on a generic level, but includes studies for salt, clay, and hard rock formations. In the following: PA studies for salt and clay formations, which are the host rock formations envisaged in Germany, are described.

Figure 3 gives a sketch of a repository in a clay formation. The waste containers are emplaced in drifts...
or boreholes (near-field), and they are entirely surrounded by a clay layer. Radionuclide transport from waste to biosphere is by diffusion within the clay and by advective flow and other transport processes in the overburden (sediments). Transport in the biosphere is modeled by a procedure, which is stipulated by the German laws [8, 9].

Figure 4 shows a similar sketch for a repository system in a salt dome. The emplacement will take place either in deep boreholes or in drifts. Far-field and biosphere are modeled similarly to the clay system.

4.2 Results of performance assessments

Representative and integrated performance assessments results are discussed for salt and clay formations as follows.

Figure 6 shows a representative result for a repository in clay from the combined projects TONI and FUNMIG [10]. The potential annual radiation exposure caused by the most relevant radionuclides is shown for a period between $1 \times 10^3$ and $1 \times 10^8$ years. The period up to $1 \times 10^6$ years is the commonly used time frame for long-term performance assessments [11]. The period up to $1 \times 10^8$ years is shown here to demonstrate when the maximum of the total dose will occur, which is at about $2 \times 10^6$ years.

The scenario for the calculations presented in Fig.6 is the reference case as discussed in Ref.[10]. The calculated potential annual radiation exposure is due to diffusion only. Radionuclides contributing most to the total dose are non-sorbing in clay or with very low sorption coefficient, like carbon, chloride or selenium. Neglecting any sorption for carbon is very conservative and is based on the assumption that a high percentage of carbon exists in organic form. Iodine is of highest importance at very late times and causes the maximum of the annual exposure either within $1 \times 10^6$ years or over the entire period of the calculation. These results are quite similar to those from a calculation performed by NAGRA for a similar system [12].

Figure 7 shows a representative result for a repository in a salt formation from a national project [13]. In general, PAs for salt formations show the interesting feature that no release occurs at all for the reference case. Thus, Fig.7 shows the model results for an altered evolution of the repository system, i.e. with large volumes of brine pockets, which are assumed to be undetected after excavation of mine and release large volumes of liquid through the emplacement sites into the near-field.
In this variant, the transport of the contaminated brine is advective, mainly caused by convergence of salt, as shown in Fig.5. All effects shown in Fig.5 are taken into account in these calculations. Although there is no sorption within the near-field, a high retardation by sorption is taken into account in the overburden. Thus, the results are in some aspects similar to the previously discussed results for clay, i.e. the most important radionuclides are those with low sorption coefficient, like iodine or caesium. Strongly sorbing elements like uranium or radium are of much less importance, although they exhibit long half-lives and thus could be of importance in long term. As the maximum of the total annual exposure is reached within $1 \times 10^6$ years, the calculations are stopped after that period.

4.3 Comparison of results for clay and salt

The main difference of PAs for both formations is that, in the reference case there is no release at all for salt, but there is always a release for clay. If releases are compared, in salt mainly advective process and in clay mainly diffusive process plays a role. Retardation occurs for clay within the formation itself, while for salt only a retardation (sorption) in the overburden can be taken into account. Nevertheless, both sorption processes yield a significant retardation of contaminants along the transport path and thus the most important radionuclides with respect to the total dose are the non-sorbing ones. The PA tools are available for both types of formations, although the tools for salt have been applied to a larger variety of assessments (Table 1) and are thus better verified.

5 Field testing and modeling of coupled thermo-hydro-mechanical (THM) processes

Field testing and comparison of experimental and modeling data are important steps for the validation of process models, which are implemented in integrated PA codes sometimes in a simplified manner.

Staff members of the GRS Department of Process Analysis are carrying out field testing for more than three decades. Starting with in-situ rock characterization and simulation tests for the salt option in the Asse underground research laboratory (URL) in the late sixties of the 20th century, GRS increased its participation in European URL research projects, e.g. for the crystalline rock option in the Åspö Hard Rock Laboratory in Sweden and the Grimsel Rock Laboratory in Switzerland, for the clay option in the Mt. Terri Project in Switzerland and the Bure URL in France.

In Germany, the Ministry of Economics and Technology (BMWi) started research on the clay option about ten years ago. Hence, in 1999, GRS joined the Mt. Terri Project and is, since then, conducting field testing in this Swiss rock laboratory in co-operation currently with 12 other project partners.

5.1 Heating experiments in clay formations

One of the experiments performed recently at Mt. Terri URL is the HE-D experiment jointly conducted by the French ANDRA and GRS. The main objectives of this experiment were to test technical equipment before being used at the Bure URL and to provide experimental field data for thermo-hydro-mechanical model validation. In this experiment (Fig.8), an electric heater with a length of 5.4 m was installed in a horizontal borehole of 30 cm in diameter and 14 m in length. The surrounding rock was heated from 15 °C to 43 °C at the heater/rock interface over the first 3 months and to 100 °C over further 8 months. A cooling phase of about 100 days followed the heating phase. During the experiment, temperature, pore water pressure, gas migration, and deformation in clay were monitored by means of more than 80 instruments installed in 24 boreholes. Thermal expansion of the heated rock was also observed. In the heated region at distances of 0.8–1.4 m far from the heater, the

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**Fig.7** Calculated potential radiation exposure for a repository in salt (altered evolution) [13].

**Fig.8** HE-D test field at Mt. Terri URL.
pore water pressure increased from 0.7–1.2 to 3–4 MPa. The THM-response of clay to heating was simulated by the involved modeling teams using different codes.

GRS applied the code CODE_BRIGHT [14] developed by the Technical University of Catalonia (UPC) in Barcelona. The theoretical framework employed in the code is presented in several papers of UPC [14–17].

The mechanical behavior of the Opalinus clay is described by the Barcelona basic model (BBM) implemented in CODE_BRIGHT, which is an elastoplastic model able to represent many mechanical features of unsaturated soils in a consistent and unified manner.

Heat transport is governed by conduction through the rock and by advective flow of liquid water and vapor. Thermal conduction is expressed by Fourier’s law.

Gas and water flow were modeled according to Darcy’s law, and the molecular diffusion of water vapor is governed by Fick’s law. The mass of water vapor per unit volume of gas is determined via the psychrometric law and the solubility of air in water is controlled by Henry’s law.

The model calculations have been performed using material parameters determined through accompanying laboratory tests [18] or taken from Ref. [19], e.g. permeability of undisturbed clay rock $k = 2 \times 10^{-20}$ m$^2$, average thermal conductivity of clay rock $\lambda = 1.7$ W/(m·K) [18].

One of the test objectives was to investigate whether the thermally induced increase of pore water pressure could lead to the generation of hydraulically effective fractures in the host rock.

Figure 9 shows the comparison of measured and predicted evolutions of the pore water pressure in the heater surroundings by coupled THM calculation. It can be seen that a maximum pore water pressure of about 4 MPa was reached in the second heating phase. Because of the high confining stresses in the heated rock, no generation of fractures could be identified either in the heating phase or in the cooling phase.

This result corroborates the assumption in PA that diffusion is the prevailing radionuclide transport mechanism in clay formations.

Furthermore, the high degree of agreement between measurement and calculation results confirms impressively the suitability of the models adopted for analyses of strongly coupled THM processes in clay.

### 5.2 Borehole sealing tests in clay formations

Currently, highly compacted bentonite buffers are studied in the frame of several concepts for the final disposal of HLW. In 2000, GRS started investigations on the suitability of moderately compacted sand/bentonite mixtures as a sealing material in clay repositories. Such mixtures may represent a reasonable alternative to highly compacted bentonite buffers, especially for the safe closing of repository rooms containing gas generating waste, since they will act as a gas vent thereby avoiding the development of undesired high gas pressures in the disposal cells. The granular material mixtures may be used as buffer and/or backfill materials in disposal boreholes or disposal drifts containing either spent fuel or vitrified HLW.

In contrast with highly compacted buffers, moderately compacted clay/sand mixtures allow gas entry/breakthrough even in the saturated state while providing a certain self-sealing potential and an adequate low permeability to water due to closure of pores by clay swelling.

![Fig.9 Evolution of pore water pressure in the test field before, during and after the heating period.](image-url)
At the first step, the sealing performance of different clay/sand mixtures with mixing ratios between 35/65 (clay/sand) and 70/30 (clay/sand) has been investigated on small samples in GRS’ geo-laboratory. The results suggested that the desired properties are best met by a mixture of 35% clay and 65% sand with characteristic material data for the water permeability of $10^{-17}$–$10^{-18}$ m$^2$ in the saturated state (which is in the same order of magnitude as that of the surrounding rock so that radionuclide migration will be a diffusion controlled process as desired) and a gas entry/gas breakthrough pressure between 0.4 and 1 MPa [20] (which is adequately low in comparison with that of the surrounding rock of 2–5 MPa so that gases will preferentially migrate away through the buffer thereby avoiding the generation of undesired high gas pressure and possible fracturing of the host rock). For comparison, the permeability and the gas entry/breakthrough pressure of mixtures of 50% clay and 50% sand, 70% clay and 30% sand were determined, which are about $1\times10^{-18}$ m$^2$ and 3 MPa, respectively.

Regarding performance assessment of repository components, the time needed to reach full saturation of the material is of major interest besides the hydraulic properties.

Therefore, as the 2nd step and before starting in-situ tests, the saturation behavior of the material was investigated in a large-scale laboratory test setup, in which steel tubes with a diameter of 0.31 m were vertically arranged. The length of the tube and the investigated seal were 2.5 and 1 m, respectively. The test setup is shown in Fig.10.

Scoping calculations were performed with the codes CODE_BRIGHT. Based on data published [16, 17, 20], the hydro-mechanical properties and parameters of the mixtures were determined by laboratory tests. Figure 11 illustrates the predicted evolution of water saturation of the 35/65 (clay/sand) mixture of 35% clay and 65% sand with an initial density of 1.94 g/cm$^3$ at a water injection pressure of 1 MPa. According to the calculation results, the saturation time amounts to about 170 days for a distance of 1 m to bottom.

The laboratory test started in early April 2005. The first water breakthrough, indicating a situation close to full seal saturation, was only observed after about 29 months in September 2007, which is much longer than predicted duration. This experimental result shows that it is indispensible to improve the certainty of the hydraulic parameters such as the water retention curve by more laboratory tests.

The water injection was stopped by reducing the injection pressure to zero after full saturation was reached, nine months later in July 2008 (Fig.12).

At this stage, the water inflow and outflow rates were equal to about 10 mL per day, yielding a water permeability of about $3\times10^{-18}$ m$^2$. This value is in very good agreement with the data determined on the small samples before. Six months later in January 2009, nitrogen gas was injected into the seal for further investigation of the gas migration of the saturated material. Measured data showed a clear start of the gas entry at a pressure of about 0.35 MPa, a value that confirms the values obtained on small samples before. Both the water permeability and the gas entry pressure measured at full saturation of the clay/sand mixture...
reveal its designed sealing properties and thus confirm the required seal function. The laboratory results supported the design of the ongoing in-situ experiments at the Mont Terri URL.

Generally, the test data obtained during the long-term sealing experiments in the laboratory provided a most valuable data basis for further calibration of the constitutive models used and improvement of self-developed PA codes.

6 Conclusions

For many years, GRS as the leading German expert organization in the field of nuclear safety has been involved in the development and application of PA tools for safety assessments of final repositories for radioactive waste.

This paper provides an overview of the status of GRS’ work. Tools are shown to be available for repositories in different host rock formations with main emphasis on tools for salt and clay formations.

Examples are given with regard to the application of these tools, i.e. computer codes that are specially developed for total system performance assessments. GRS participated in several national safety cases of repositories for low-level waste, mainly in salt formations.

Furthermore, examples are given on experimental laboratory and field investigations for the testing and improvement of process level codes specifically suitable for the numerical simulation of coupled THM processes in repository systems.

Many participations in international benchmark exercises confirmed the high level of proficiency of the PA tools developed and applied by GRS.

At the moment, a focus of German R&D (research and development) work is in the demonstration of completeness of PA tools to establish a safety case for a high-level waste repository. In this respect, the codes of GRS are checked and methods for a systematic development of scenarios are under debate. At the first step, GRS participated in a project to develop a catalogue of features, events, and processes (FEP) of a German HLW repository in rock salt.

Future work of GRS will focus on the improvement of its PA tools for the clay option, including the consideration of fracture systems as well as the testing of clay-sand mixtures under the impact of higher temperature representing the near-field conditions in a HLW repository.

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References