Underground waste disposal safety research: development and application of analytical tools and methodologies for the safety case

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Abstract:

The safety analysis computer codes of GRS can be used to model various developments of a repository for hazardous wastes in deep geological formations. The modular structure of the software package enables a simple adaptation to project- and site-specific requirements. The program modules enable the calculation of pollutant releases from the wastes and the transport in the immediate vicinity of the wastes, the transport in the geosphere and the radiation exposure under consideration of all exposure pathways. Their relevant features are summarised and current developments regarding the adaptation, development and use for concrete applications of models and tools are described.

1. INTRODUCTION

The final disposal of hazardous wastes in deep geological formations requires a well-founded system understanding to prevent potential risks from the outset by adequate technical concepts and design features or to counteract them as far as possible. The hazardous wastes, for which disposal in the deep underground is mandatory or envisaged, embrace radioactive wastes, chemical-toxic wastes and carbon dioxide, respectively. With the aim to assess and predict the long-term confinement of such wastes with regard to the safety of man and the environment and over geological time scales, GRS develops methods and procedures for safety analyses that are already applied for site selection and repository planning. The main technical design features and safety-relevant components with their material properties are modelled numerically. On this basis, GRS simulates the evolution of a repository under normal conditions of the surrounding rock mass and the effectiveness of the different technical and geotechnical barriers.
From the calculated behaviour of waste species safety indicator values are derived that are compared with regulatory limits. Possibilities for a system optimisation can be identified by additional performance indicators. In case of radioactive wastes adherence to regulatory limits is demonstrated on the basis of individual dose rates which are derived from calculated radionuclide concentrations in the biosphere.
However, there are some uncertainties regarding the long-term development of a repository and the prediction as to system-specific processes. Therefore, additional scenarios are considered and load cases defined which may result from events that cannot be fully excluded. In this respect, it is relevant for safety analyses that the repository is a complex geological-technical system, especially under the impact of heat and humidity, where a number of coupled processes are time-varying and, to some extent, non-linear.

2. SAFETY ANALYSIS PROGRAM SYSTEM

The safety analysis computer codes of GRS can be adapted to model the evolution of a repository both under normal conditions and under accident conditions that cannot be fully

excluded. They are continuously further developed and tested application specifically and they are used both for deterministic and probabilistic analyses of the integral repository system or of repository subsystems.
The repository system is conceptually divided into three subsystems, i.e. the near field, the far field or geosphere, and biosphere, respectively. For each subsystem dedicated program modules for different rock formations and disposal configurations are available that can be combined via standardised interfaces (see Figure 1) within a shell program which contains also routines for data input and result output. Originally, all routines for the various repository subsystems were implemented within one code called EMOS, therefore, the software package is still referred to as EMOS.
The modular structure of the safety analysis tools enables the adaptation of these modules to project- and site-specific requirements. The module CLAYPOS, currently being developed for a repository in argillaceous rock, describes the release from wastes and the one-dimensional diffusive transport in the undisturbed host rock. Thus, this model can be used for modelling the transport behaviour in argillaceous rock in the near and far field. The biosphere modules calculate the individual dose rates on the basis of radionuclide concentrations (EXCON) or on the basis of radionuclide fluxes (EXMAS).

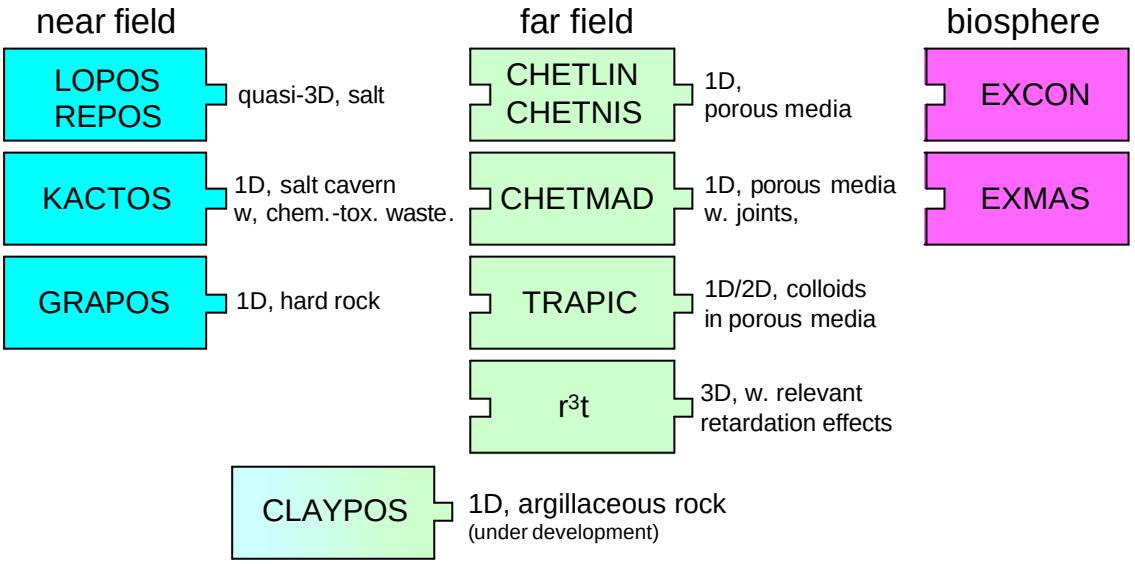

Fig. 1: Available program modules for integrated long-term safety analyses

The program modules enable the calculation of pollutant releases from the wastes and the transport in the immediate vicinity of the wastes, the transport in the geosphere and the radiation exposure under consideration of all exposure pathways. All modules consider the radioactive decay of the radionuclides. Relevant further characteristics of selected modules for modelling the release and transport of radionuclides or pollutants in the near and far field are summarised in Table 1.

Tab. 1: Relevant characteristics of selected EMOS modules for modelling the release and transport of radionuclides or pollutants in the near and far field

Processes	**LOPOS**	**GRAPOS**	**CLAYPOS**	**CHETLIN CHETNIS**	**CHETMAD**	**TRAPIC**	**r^3t**
Maximum dimension	3D*	1D	1D	1D	1D	2D	3D
Mobilisation	✓	✓	✓				
Container failure, container corrosion	✓	○	○				
Advection	✓			✓	✓	✓	✓
Diffusion	✓	✓	✓	✓	✓	✓	✓
Dispersion	✓			✓	✓	✓	✓
Solubility limits	⊗	⊗	⊗				⊗
Speciation	○	○	○				○
Complex formation							⊗
Equilibrium sorption	✓	✓	✓	✓	✓	✓	✓
Surface complex formation							○
Ion exchange							○
Sorption kinetics						✓	✓
Diffusion in immobile pore waters					✓		✓
Colloid-borne transport					⊗	⊗	⊗
Gas formation, gas transport	⊗						

✓ = Process is modelled completely, ⊗ = Process is modelled in a simplified manner, ○ = Process is implemented within the framework of current projects, gryed fields = modelling of the process within the module is not useful.
* = quasi 3D, realised by linkage of several 1D sections in different directions

3. APPLICATIONS

Integrated long-term safety analyses are performed by GRS with different objectives. These are the

- assessment of processes and parameters with regard to necessary research and development activities,

- support in site selection and steering of site exploration,
- assessment and optimisation of technical repository concepts, and
- safety assessment in the licensing procedure.

The software package EMOS has already been used in numerous international and national studies, see Table 2. EMOS was and is used in all licensing procedures for sites for the final disposal of radioactive wastes in Germany. Most of the studies were performed for radioactive wastes in saliniferous rock. Sedimentary rock was analysed within the framework of activities for the Konrad mine, and hard rock within the framework of the EU SPA project. The EU projects PAGIS, PACOMA, EVEREST and SPA belong to the category of research and development activities, the projects PSE and SAM/SEK to the category of research and development activities and optimisation of technical repository concepts.

Tab. 2: Use of the EMOS software package in international and national studies.

Study	Period of time
PSE: *Project safety studies final disposal*	1980 – 1984
KONRAD: *Safety analysis for the application procedure for the Konrad mine*	1984 – 1986
PAGIS: Performance assessment of geological isolation systems for radioactive waste	1982 – 1987
PACOMA: Performance assessment of confinements for medium-level and alpha-contaminated waste	1987 – 1991
SAM/SEK: System analyses dual-purpose repositories/ *concepts for final repositories*	1987 – 1992
EVEREST: Evaluation of elements responsible for the effective engaged dose rates associated with the final storage of radioactive waste	1992 – 1994
Development of a near-field model for long-term safety analyses of salt caverns with chemical-toxic wastes	1993 – 1996
ERAM: Morsleben repository for radioactive wastes	since 1993
SPA: Spent fuel performance assessment	1996 – 1999
LASI: Renewed long-term safety analysis	1996 – 1999
ASSE: *Safety analysis for decommissioning and closure of the Asse mine*	since 2000

4. FURTHER DEVELOPMENTS

In general, the safety analysis program modules model processes in a simplified way, mainly to make the complexity of processes manageable for a numerical simulation. In this respect, it has to be demonstrated that the simplified assumptions are admissible. Likewise, it has to be proven that the model results, as far as influenced by simplifications, are on the safe side, i. e. that the calculated potential radiation exposure is overestimated.
These proofs have to be furnished on the basis of an in-depth system understanding together with newly developed or improved models at the process level. In this respect,

newer findings on processes not considered in long-term analytical calculations before have continuously to be considered and assessed for their relevance. Thus, safety-analytical research and development activities concentrate particularly on such aspects.
In the integrated long-term safety analyses to date, the pollutant transport through the geosphere has generally been calculated one-dimensionally to save calculation time, on the one hand, and, on the other hand, because there was no computer code available that considers all relevant interactions for large three-dimensional model areas at the same time. In future safety studies, one-dimensional transport programs will further be applied in probabilistic analyses to keep the calculation time within practicable limits. However, for the validation of a simplified geometrical model, detailed and realistic deterministic analyses have to be performed, in particular three-dimensional calculations for large areas under consideration of all relevant interaction effects. From such three-dimensional models, relevant input parameters for one-dimensional model calculations, e. g. dilution factors and transport cross-sections, can be derived. By means of three-dimensional transport calculations, an in-depth understanding of the consequences of the relevant retention effects for the pollutant transport can be achieved and the influence of the geological heterogeneities can be analysed. However, the procedures to date on the determination of the individual representative dispersion pathways by means of particle tracking only considered the advective transport.
With the transport program r^{3}t (**r**adionuclides, **r**eaction, **r**etardation and **t**ransport), a suitable tool is now available at GRS which is able to consider the relevant retention effects for large, heterogeneous, three-dimensional model area. During its development – as was the case with the d^{3}f computer code – adaptive procedures, by which the grid is locally refined or coarsened according to the respective physical processes, and effective solution algorithms were realised for linear and non-linear problems for parallel calculation architectures. The geometrical solution of heterogeneities is reached by the application of unstructured grids, using effective solution algorithms for large equation systems.
Additional aspects, currently dealt with within the framework of research and development activities on the further development of safety analysis methods, concern, in particular,

- the consideration of the speciation of radionuclides and other pollutants with regard to their mobilisation, transport and sorption behaviour,
- the relevance of the colloid-borne transport,
- gas formation and gas transport, and
- the change of hydraulic parameters resulting from the waste heat input or chemical transformations.

The mobilisation of the radionuclides and other pollutants from the wastes and their transport in the near and far field is decisively influenced by the chemical environment which, among other things, determines the solubility and sorption of the pollutants. Since the chemical environment may change locally due to inflow and outflow of aqueous solutions, a time-dependent modelling of the process in long-term safety analysis calculations is necessary. Moreover, dissolution and reprecipitation processes and changes in the composition of the aqueous phase may lead to gas formation and volume effects which have a retroactive effect on the transport processes. Until now, however, such chemical processes have only been modelled in EMOS in a very simplified way. At present, approaches are explored in different projects to find out how program modules can be coupled with geochemical speciation projects, such as PHREEQC or ChemApp, in an appropriate manner. Since these codes for the geochemical modelling are also very calculation intensive, there is a great demand for optimisation of the algorithms for the coupling of the geochemical codes with the program modules.
Moreover, there is additional demand for research and development in order to

- enable the consideration of processes not considered before,
- improve conceptual models based on simplified assumptions,

- refine mathematical methods, and
- implement approaches for new safety analysis models, such as the consideration of risk values or the use of suitable safety and performance indicators.

Most of these topics are dealt with in current research projects.

5. OUTLOOK

The scientific and technological state-of-the-art regarding long-term safety analysis methods advances continuously at the national and international level. The understanding of the processes responsible for pollutant release from the wastes as well as transport and retention in the deep underground up to the biosphere becomes increasingly detailed and better. In this respect, laboratory and in-situ experiments of GRS make an indispensable contribution. The adaptation, development and use for concrete applications of models and tools required for integrated safety assessments on the basis of a comprehensive system understanding remains to be the most important task of the Long Term Safety Analyses Department also in the future. This includes the application of the methods and the available tools to issues in non-nuclear fields, such as the storage of carbon dioxide in the deep underground.