The virtual underground research laboratory

The VIRTUS software platform (virtual underground laboratory in salt) is being developed. In combination with specific process-level codes, VIRTUS provides a powerful tool for simulating and visualizing the coupled thermal-hydraulic-mechanical processes occurring in a repository or underground laboratory in the context of geology and mine structure.
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In the course of the operation of nuclear power plants heat-producing radioactive waste is generated which, according to international consensus [1] and the concepts most countries using nuclear power are developing, should be disposed of in deep geological formations. In different countries, different host rocks are considered depending on their respective geological situations. In general, crystalline rock, clay rock and salt formations are under investigation. The latter two are favoured in Germany.

For constructing a repository and for ensuring the safe containment of the nuclear waste over very long time periods, it is necessary to have profound knowledge about the material behaviour of the host rock itself, and the system of waste forms, and technical components such as sealing structures for boreholes, drifts, and shafts, and the rock. In order to obtain this knowledge, some countries operate underground rock laboratories (URLs), which are also recommended by NEA guidelines [2].

In Germany, rock salt has been intensively investigated over several decades as a potential host rock. An underground laboratory in salt, however, is not available at this time. In order to compensate for this deficit, and to provide a powerful instrument for the evaluation of the processes occurring in a repository, and to test repository concepts, the idea of a virtual underground laboratory in salt (VIRTUS) was developed. VIRTUS combines powerful visualization software for geological models and results of numerical simulations with functions for management of material and project data. Thus, VIRTUS is a software platform and data hub at the same time.

For reliably predicting the coupled thermal-hydraulic-mechanical (THM) processes occurring in a repository, a profound knowledge of material behaviour is required. Data acquired during more than 30 years of repository research in salt are evaluated in the frame of the VIRTUS project and stored in a consolidated database, where they are available as input data for numerical simulations. These data include thermal, hydraulic and mechanical properties for different types of rock as well as waste forms and geotechnical components, such as backfill materials or sealing structures. In the process of the evaluation, data quality is assessed and shortcomings are determined.

The numerical simulations are performed outside of VIRTUS using so-called process-level codes (usually finite element or finite difference codes), which have been developed specifically for this task. Such codes have been used, improved, and validated in many national and international projects [3-6], to name a few.

Numerical models and material parameters have been established and validated; this, however, does not imply that no further experimental studies are needed in the future. Material properties can be site-dependent and will have to be determined at the actual repository location; experiments will have to be performed and simulated by process level codes to show that the actual coupled behaviour can be captured and predicted. Thus, VIRTUS cannot replace future experimental work. For a given repository site, VIRTUS will facilitate:

- Design of meaningful experiments
- Comparison of the outcome of simulations with actual measured data
- Comparison of simulations with different codes for benchmark purposes
- Comparison of simulation variants for optimization purposes
- Evaluation of simulation results to make sure that safety criteria (maximum temperature, acceptable stress states) are met
- Design of an actual repository structure in a given geology.

VIRTUS is developed to have a serviceable tool at hand once a potential repository site or a set of such sites have been selected. This tool can then be used by research organizations to plan their experiments, by the waste management organization to design the repository so that it meets safety requirements, and by the regulatory authority for help in their assessment.

To sum up, the most important objectives of the current VIRTUS project are:

- To develop the components and tools of a virtual underground laboratory or repository in rock salt for visualization and interpretation of the results of numerical simulations in context with geology and mine structure
- To provide a consolidated and quality-assured THM database for numerical simulation of URL experiments and repositories
- To perform prototypical simulations of

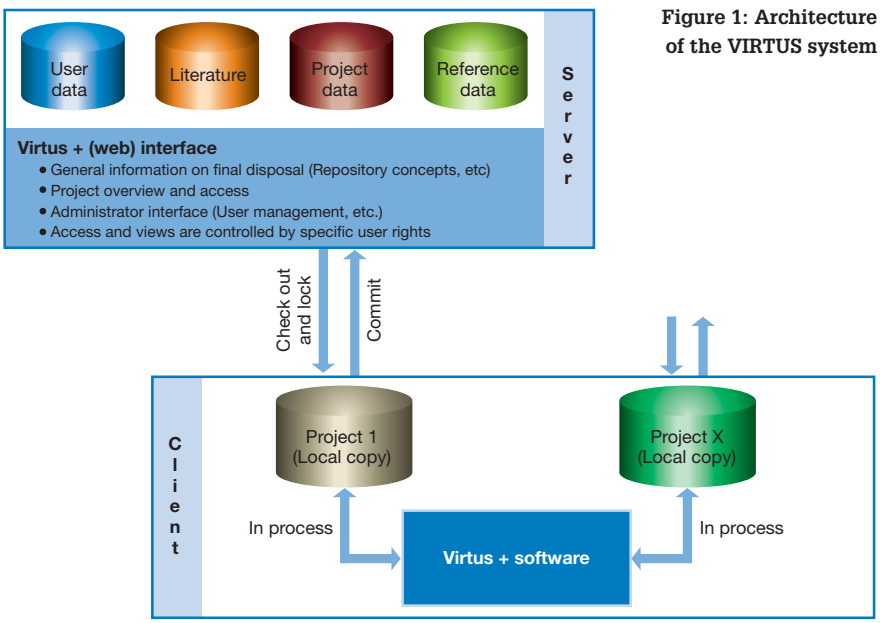
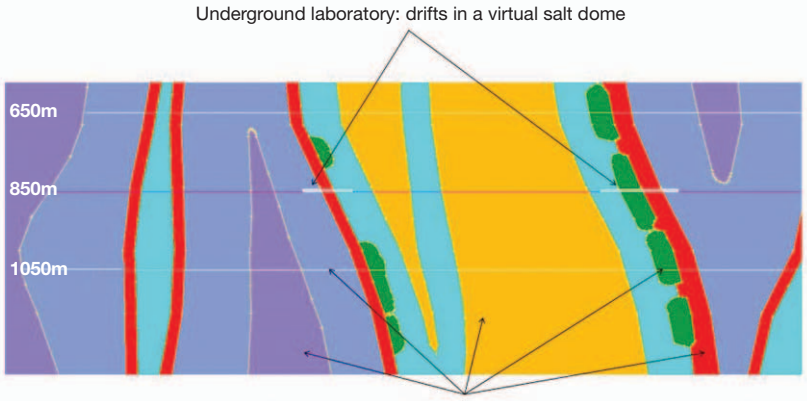


Figure 1: Architecture of the VIRTUS system

Figure 2: Vertical section of a virtual salt dome with typical saliferous series



selected URL and repository configurations with dedicated process level codes (PLC). The project is financed by the federal ministry for economy and technology (Bundesministerium für Wirtschaft und Technologie (BMWi)); the current project phase started in November 2010 and runs until October 2013. Three organizations with long experience in repository research have joined forces for the implementation of VIRTUS: technical consultancy firm Gesellschaft für Anlagen- und Reaktorsicherheit (GRS), the German geological survey (Bundesanstalt für Geowissenschaften und Rohstoffe (BGR)), and repository construction firm DBE Technology GmbH. All three organizations are involved in the conceptual design, the evaluation of repository research data, and the numerical simulations. The Fraunhofer Institut für Fabrikbetrieb und –automatisierung (IFF) was contracted by GRS for development and implementation of the software platform.

The VIRTUS system is implemented in a server-oriented architecture; that is, there will be local VIRTUS software platforms and a server that will provide specific services (Figure 1).

The main task of the local component (client) is to provide a user interface for modelling, evaluation, and visualization of the experiments and their results, while the server handles user administration and access control, project administration including version control, the THM database, the literature database, and the administration interface. For implementation and testing of the server architecture a local test environment was constructed at Fraunhofer IFF. The server will be ported to GRS after completion of implementation and testing.

A typical workflow

VIRTUS functionalities include import of geological models and mine structure models, generation and editing of mine structures, functions to correct, improve or simplify these surface models, define cut-outs for export to process-level codes used for numerical simulations, and import and visualization of the simulation results. These functionalities are explained below in a typical workflow.

Geological model

Geological models are generated by BGR using the code openGEO [7], of which it is a major user. openGEO is used to construct three-dimensional models of geological-tectonic reservoirs. These reservoir models include all available information: geological, mineralogical-chemical, or geophysical. With openGEO it is possible to create highly complex models of very small as well as very large scales and to combine them to a consistent overall model. The openGEO models are the basis for planning, archiving and further modelling calculations. Figure 2 shows a vertical section of a typical saliferous formation model, which is used for the prototypical model simulations. For the transfer of geological models between openGEO and VIRTUS an XML-based data format developed by BGR is used.

A geological model imported in VIRTUS intended to be used for numerical simulations has to comply with several quality requirements in order to enable a successful generation of a finite element mesh. These include:

- Tightness-of-fit of each geological body needs to be assured
- Interpenetration of geological bodies has to be ruled out
- The ratio of areas of large and small surface triangles has to remain within a certain range, depending on context
- The interior angles of surface triangles should be balanced, and not go below a minimum of five degrees.

Furthermore, it is convenient, but not compulsory, to describe the surface of

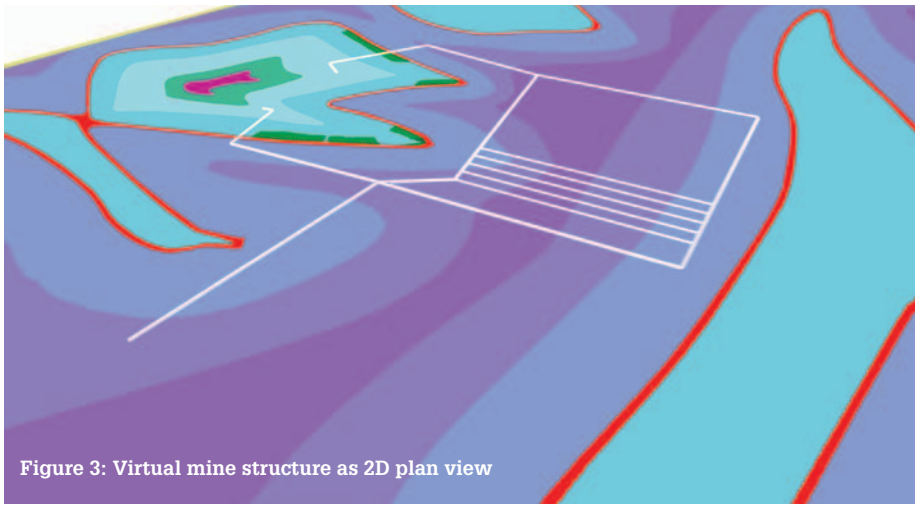


Figure 3: Virtual mine structure as 2D plan view

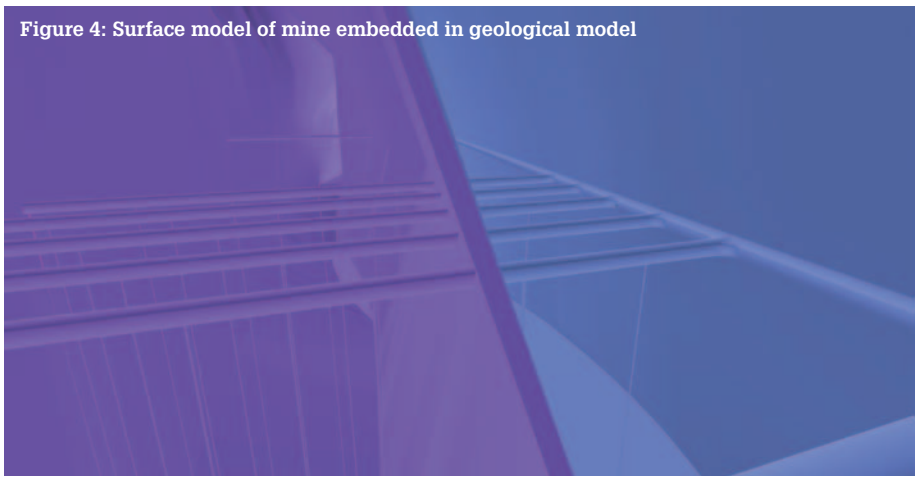


Figure 4: Surface model of mine embedded in geological model

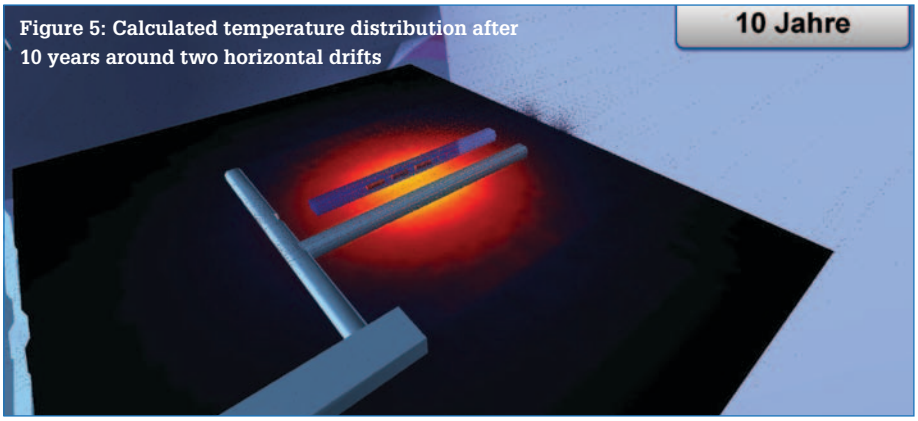


Figure 5: Calculated temperature distribution after 10 years around two horizontal drifts

geological bodies with as few triangles as possible in order to facilitate subsequent finite element mesh generation. openGEO performs an interpenetration check; after import into VIRTUS additional checks and corrections of the surface mesh are performed.

Mine structure

Besides the characterization and representation of geological structures, actual mine structures are required for numerical simulation of experiments on repository safety. VIRTUS provides methods and user interfaces for generating such structures directly in context with the geology. The mine structure is represented by an undirected graph and can be compiled with combinations of drifts, intersections and shafts. Figure 3 shows the mine layout used for the prototypical simulations as a plan view in a horizontal section of the virtual geology. The individual drifts are characterized by drift axis and cross section. Typical default cross sections are implemented in VIRTUS; others can be defined and added by the user. Based on the defined mine structure, a three-dimensional surface model is generated automatically. Details of corner arcs at bends, intersections or drift ends are parameterized and are considered during generation of the 3D geometry. A part of the mine structure as defined in Figure 3 is shown as a surface model in Figure 4, together with the surrounding geology. Note the vertical boreholes below the parallel drifts which are intended for simulated waste emplacement. Besides generation of the mine structure within VIRTUS, there is also the possibility to import existing mine structures created with CAD programs.

Prior to export, the surface model of the mine structure and the geological model have to be bound together; the resulting surface model has to comply with the same quality criteria as geological models. Accordingly, mesh healing and re-meshing algorithms can be applied to the combined model.

Export to process-level codes

In general, the complete model of the geology and the mine structure is too large for use with simulation tools; also, a certain experiment will not affect the whole model. It is reasonable to use only a part of the model for the PLC simulation. Accordingly, three-dimensional cut-outs of the surface model can be defined and exported to the pre-processors of the PLC via an XML data format or others (such as IGES). In addition to the geometrical data, material data required as input for the respective numerical simulation are exported to the PLC. These data include thermal, hydraulic and mechanical property data for host rock, waste forms and geotechnical components, such as backfill materials or sealing structures. Data range from constant values for physical quantities to parameters of complex constitutive laws describing for example temperature- and stress-dependent creep of rock salt.

Numerical simulation outside VIRTUS

Finite element mesh generation from the exported surface mesh and numerical model simulation are performed by the PLC outside VIRTUS using codes specifically developed for this task. Each project partner uses different codes: GRS employs the PLC CODE_BRIGHT [8] developed by the Technical University of Barcelona, BGR uses the proprietary development JIFE [9-11] and DBE TEC uses the commercially-available FLAC3D code [12]. All three codes are suitable to simulate thermal, hydraulic and mechanical or coupled (TH, TM, HM or THM) problems. Obviously, the calculation effort increases on the one hand with increase of the number of process classes considered and with model size on the other. At this time, three virtual experiments with different emphases are under preparation. Each

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of the three partners will be simulating one of these experiments with their modelling tool. The objective of these simulations is to test and demonstrate the visualization abilities for realistic application cases, rather than perform actual calculations. The simulations are:

- An isothermal mechanical calculation of a drift passing through different types of rock (rock salt, potash salt, anhydrite), illustrating their different mechanical behaviour. In salt materials, mechanical stresses are reduced with time due to their creep behaviour, while in the elastic mineral anhydrite stresses concentrate. The quantities to be visualized are deformations and stresses. This simulation is performed by BGR.
- A pure thermal calculation of an array of emplacement boreholes (see Figure 4) performed by DBE TEC, showing the temperature evolution in the surrounding rock. The calculation model will be rather large, but the complexity of the calculation is reduced, because only thermal effects are considered. Output quantities are temperature and heat flow.
- A coupled thermal-mechanical calculation of a heated drift in rock salt approaching a potash layer and anhydrite blocks. This GRS simulation explores the mechanical response of the rock to heating, with coupled phenomena like thermally-induced stresses and accelerated creep due to increased temperature. Both thermal and mechanical quantities are the outputs.

Import and visualization of results

In order to facilitate the import of first simulation results from the PLC, an interface for the native output format of CODE_BRIGHT was implemented in VIRTUS. Figure 6 shows the visualization of a thermal simulation of two heated drifts in rock salt performed early in the project. (In the future this import/export data format will be replaced by a jointly-developed binary format now used by VIRTUS internally).

The type of data actually visualized depends on the simulation case that has been calculated. VIRTUS is prepared to visualize thermal data, such as temperature and heat flow, hydraulic data, such as liquid or gas pressure, flow and saturation, and mechanical data, such as stresses, deformations, strains and porosity. The visualized data can be scalar quantities (temperature, porosity), vectors (displacements), or tensors (stress). Scalars can be represented by scatter plots, section planes or iso-surfaces. Vectors or tensors can be represented as arrows or triads (although suitable selection and scaling methods are needed to obtain a meaningful visualization). Additional post-processing functions include, for example, calculation of absolute values or determinants, principal stresses, and stress invariants.

Prospects

Most of the VIRTUS features described above are already implemented. The PLC simulations are in preparation. During the coming months, they will be performed and the entire system will be tested by the project partners. A VIRTUS prototype is scheduled to be available at the end of 2013. In the current project phase, VIRTUS has been developed as a virtual underground laboratory in salt. All the VIRTUS components are, however, not restricted to use in a special formation. By extending the database to other rock types and including their specific requirements, it can be used for any type of host rock. Its capabilities to quickly generate virtual mine structures and provide surface models for numerical simulations, as well as its visualization capabilities, will make it a useful tool in the development and comparison of repository concepts. ■

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