Virtual Underground Laboratory for Rock Salt – VIRTUS – 14247

Klaus Wieczorek *, Steffen Masik **, Joachim Behlau ***, Christian Mueller ****
* Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH
** Fraunhofer Institut fuer Fabrikbetrieb und –automatisierung (IFF)
*** Federal Institute for Geosciences and Natural Resources (BGR)
**** DBE Technology GmbH

ABSTRACT
In the frame of a joint project financed by the German Federal Ministry of Economics and Technology (BMWi), the VIRTUS software platform (virtual underground laboratory in salt) is developed. In combination with specifically developed 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. This will make it a useful tool for institutions involved in design and implementation of a repository as well as for research organizations and regulators for evaluation and information of the public.

INTRODUCTION
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 geologic formations. In different countries, different host rocks are considered as a consequence of their respective geologic situations.

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

In Germany, rock salt as a potential host rock has been intensively investigated over several decades. An underground laboratory in salt, however, is not available at this time. In order to compensate for this drawback by providing a powerful instrument for the evaluation of the processes occurring in a repository, the idea of a virtual underground laboratory in salt (VIRTUS) was developed.

VIRTUS CONCEPT AND OBJECTIVES
For the development of VIRTUS, the three major companies involved in repository research, the Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH, the Federal Institute for Geosciences and Natural Resources (BGR), and the DBE Technology GmbH, joined forces with the Fraunhofer Institut fuer Fabrikbetrieb und –automatisierung (IFF) with their experience in software development.

VIRTUS combines a powerful visualization software for geologic models and for result data from numerical simulations with functions for management of material and project data. Thus, VIRTUS is a software platform and data hub at the same time. The institutions participating in repository projects receive a tool for analyzing and conspicuously visualizing the complex safety-relevant processes occurring in an underground laboratory or a repository, which also helps to effectively plan and check repository layouts within the potentially complicated geologic structures.

Profound knowledge of the material behavior is required for reliably predicting the coupled thermal-hydraulic-mechanical (THM) processes occurring in a repository. Literature accumulated during more than 30 years of repository research in salt is evaluated in the frame of the VIRTUS project and relevant information is stored in a consolidated database, where it is available as input data for numerical simulations. These data include thermal, hydraulic and mechanical property values for the different types of rock as well as waste forms and geotechnical components, e.g., 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 in the frame of other projects. Such codes have been used, improved, and validated in many national and international projects, like the European Community projects BAMBUS I [3] and II [4], THERESA [5], and a German project addressing the comparison of constitutive models for the mechanical behaviour of rock salt [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. Material properties can be site-dependent and will have to be determined at the actual repository site; 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 for planning their experiments, by the waste management organization to design the repository so that it meets the 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 selected URL and repository configurations with dedicated process level codes (PLC).

While, in the current phase, VIRTUS is limited to a virtual salt geology and material data for a repository in salt, this is no general restriction. VIRTUS is developed in a way to enable adaption to other host rock types. By extending the database to other rock types and including their specific requirements regarding the VIRTUS functionalities, it can be used for any type of host rock.

The project is financed by the federal minister for economy and technology; the current project phase started in November 2010 and runs until April 2014.

ARCHITECTURE OF VIRTUS

The VIRTUS system is implemented with a service-oriented architecture, i.e. there will be local VIRTUS software platforms and a server that will provide specific services. Figure 1 gives an overview of the entire system.

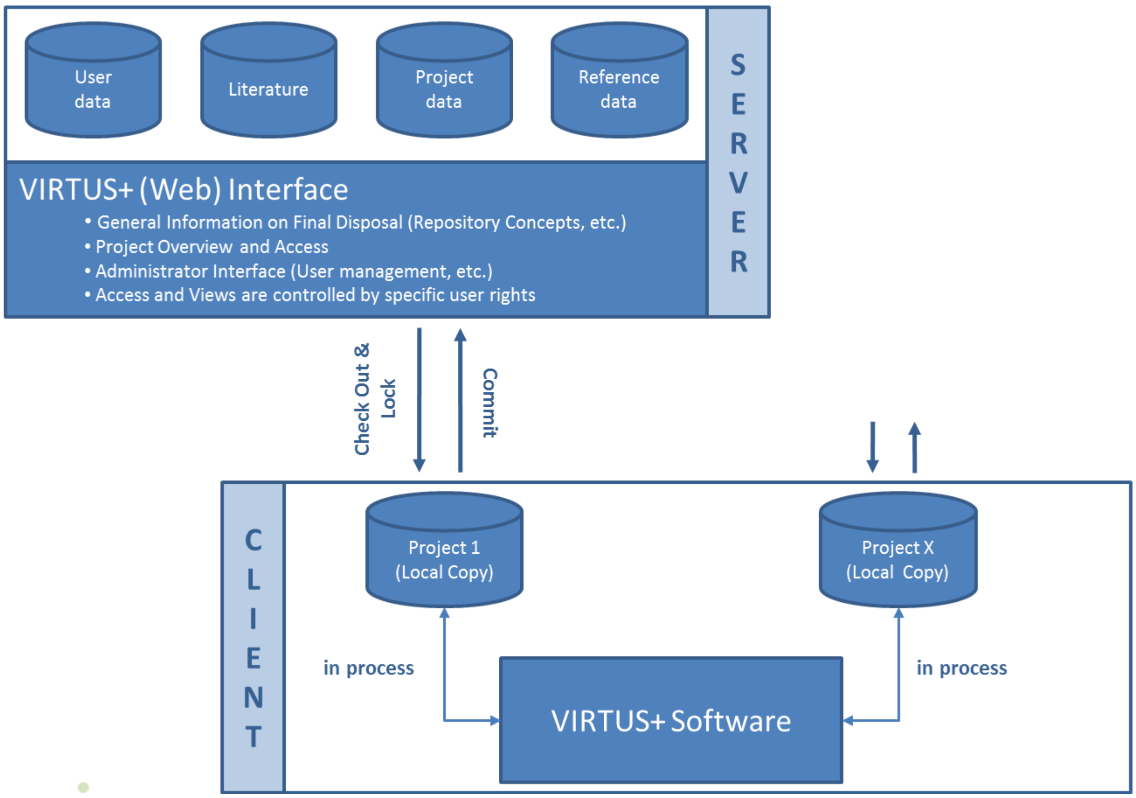

Fig. 1. Architecture of the VIRTUS system

Main task of the local component (client) is to provide a user interface for modeling, evaluation, and visualization of the experiments and their results, while the server takes the following tasks:

- User administration and access control
- Project administration including version control
- THM database, literature database
- 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.

VIRTUS FUNCTIONALITY: A TYPICAL WORKFLOW

The VIRTUS functionalities include import of geologic 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 following a typical workflow:

- Import of the geologic model
- Generation of the mine structure and integration in the geology
- Export of different model parts to the process-level codes (PLC)
- Finite element mesh generation and simulation calculation by the PLC (outside VIRTUS)
- Import and visualization of the simulation results in VIRTUS

Geologic Model

VIRTUS is prepaped to directly read geologic models generated by BGR using the code openGEO [7]. BGR is one of the main openGEO users and is significantly involved in its advancement. openGEO is used to construct three-dimensional models of geologic-tectonic reservoirs. These reservoir models include all available information – geologic, 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 modeling calculations.

Figure 2 shows a section of a typical saliniferous formation model which is used for the prototypical model simulations. For the transfer of geologic models between openGEO and VIRTUS an xml-based data format developed by BGR is used.

A geologic model imported in VIRTUS 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 the following requisites:

- Closeness of each geologic body needs to be assured.
- Interpenetration of geologic bodies has to be excluded.
- The area ration of large and small surface triangles has to remain in a context-dependent range.
- The inner angles of the surface triangles should be balanced, they should not go below a minimum value of five degrees.

It is further convenient, but not compulsory, to describe the surface of geologic bodies with as few triangles as possible in order to facilitate the subsequent finite element mesh generation.

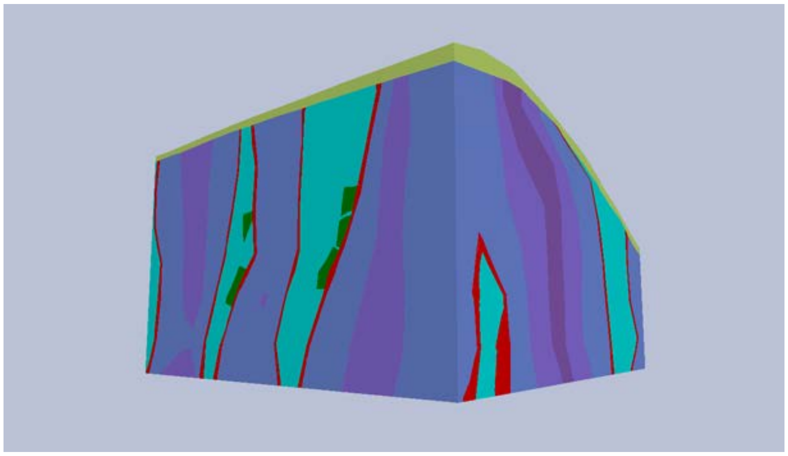

Fig. 2. Section of a virtual salt dome with typical saliniferous series: rock salt (blue), potash salt (red), sulfates (green), cap rock (yellow)

A check of interpenetration is already performed by openGEO. After import into VIRTUS additional checks and corrections are performed. In order to obtain a surface mesh usable for finite element mesh generators, IFF has developed the following functions:

- Removal of minimal triangles (zero-area triangles)
- Rectification of surface normals (improvement of visualization)
- Simplification of surface triangle meshes (polygon reduction) while keeping the model shape (mesh healing)
- Regularization of surface meshes (re-meshing)

The algorithms for simplification and regularization of triangle meshes are geared to concepts of recent publications in computer graphics research and were developed further according to the requirements of VIRTUS. Figure 3 shows a cuboid section from the geologic model after various steps of improvement.

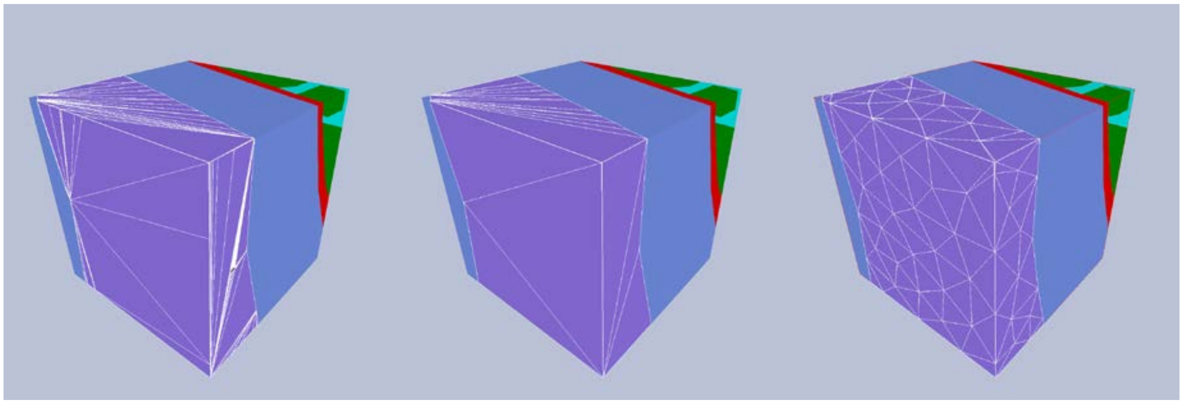

Fig. 3. Cuboid section from the geologic model showing the surface mesh of a salt layer (blue). Left: original mesh, center: simplified mesh, right: mesh after regularization

Mine Structure; Combination with the Geologic Model

Besides the characterization and representation of geologic structures, the actual mine structures are required for numerical simulation of experiments regarding repository safety research. Therefore, 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 by adequate combinations of drifts, intersections, shafts, and boreholes. 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 so-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 4 is shown as a surface model in Figure 5, together with the surrounding geology. Note the vertical boreholes below the parallel drifts which are intended for simulated waste emplacement.

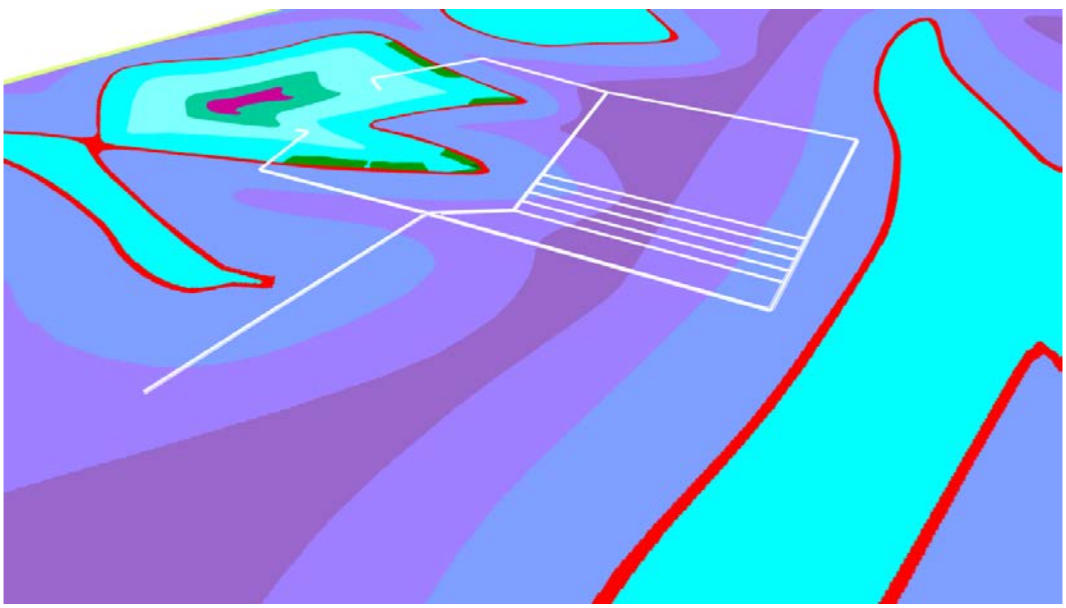

Fig. 4. Definition of a virtual mine structure

Besides generation of the mine structure within VIRTUS, there is also the possibility to import existing mine structures created with CAD programmes. The structure shown in Fig. 6 was used for an early test simulation (see section on import and visualization of simulation results).

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

Fig. 5. Surface model detail of the mine structure embedded in the geology

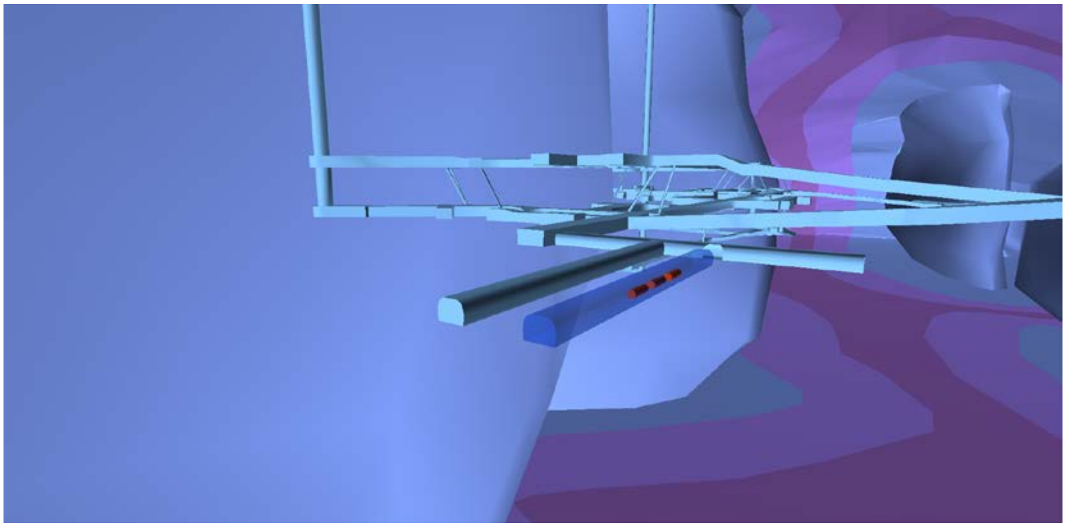

Fig. 6. 3D geometry of an imported virtual mine structure

Export of Model Cut-outs and Material Data to Process-level Codes

In general, the complete geology model and the mine structure is too large for use with simulation tools; on the other hand, a certain experiment will not affect the whole model. Therefore, 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. In addition to the VIRTUS-specific xml data format, other formats (e.g., iges) which can be interpreted directly by the PLC are supported, so that an xml interface of the PLC is not mandatory.

Besides the geometric data, also the material data required as input for the respective numerical simulation are exported to the PLC from the VIRTUS database. Material 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, e.g., 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. These codes have been specifically developed for this task. The project partners are using different codes which can all be used with VIRTUS. GRS employs the PLC CODE_BRIGHT [8] developed by the Technical University of Barcelona, BGR uses their proprietary development JIFE [9, 10, 11] and DBE TEC uses the commercially available code FLAC3D [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 regarding their complexity are under preparation. Each of the three mentioned partners will be simulating one of these experiments with their modelling tool.

For the current development phase of VIRTUS, the objective of these simulations is to test and demonstrate the visualization abilities for realistic application cases, rather than perform actual optimization or benchmark calculations. The cases are

- An isothermal mechanical calculation of a drift passing through different types of rock (rock salt, potash salt, anhydrite), illustrating their different mechanical behavior. In salt materials, mechanical stresses are reduced with time due to their creep behavior, while stresses concentrate in the elastic anhydrite. 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 Fig. 5) 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, performed by GRS. This 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 as mentioned for the other two cases are output.

Import and Visualization of Simulation 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. Currently this import/export data format is replaced by a jointly developed binary format which is already used by VIRTUS internally. The advantages of the binary format are the increased reading rate and especially the lower memory demand of the simulation results.

The type of data actually visualized depends on the simulation case that has been calculated. VIRTUS is prepared to visualize thermal, hydraulic, and mechanical data. As described in the previous section, thermal data include temperature and heat flow, and mechanical data are, e.g., stresses, deformations, strains, porosity. Hydraulic output data will include liquid or gas pressure, flow, saturation.

The result data visualized can be scalar quantities (e.g., temperature, porosity), vectors (e.g., displacements), or tensors (e.g., stress). Scalars can be represented by scatter plots, section planes or iso-surfaces. For vectorial or tensorial quantities arrow and triad representations are available. For the latter, suitable selection and scaling methods are needed to obtain a meaningful visualization. Of course, vector or tensor components can be represented like scalars. Additional post-processing functions include, e.g., calculation of absolute values or determinants, principal stresses, and stress invariants.

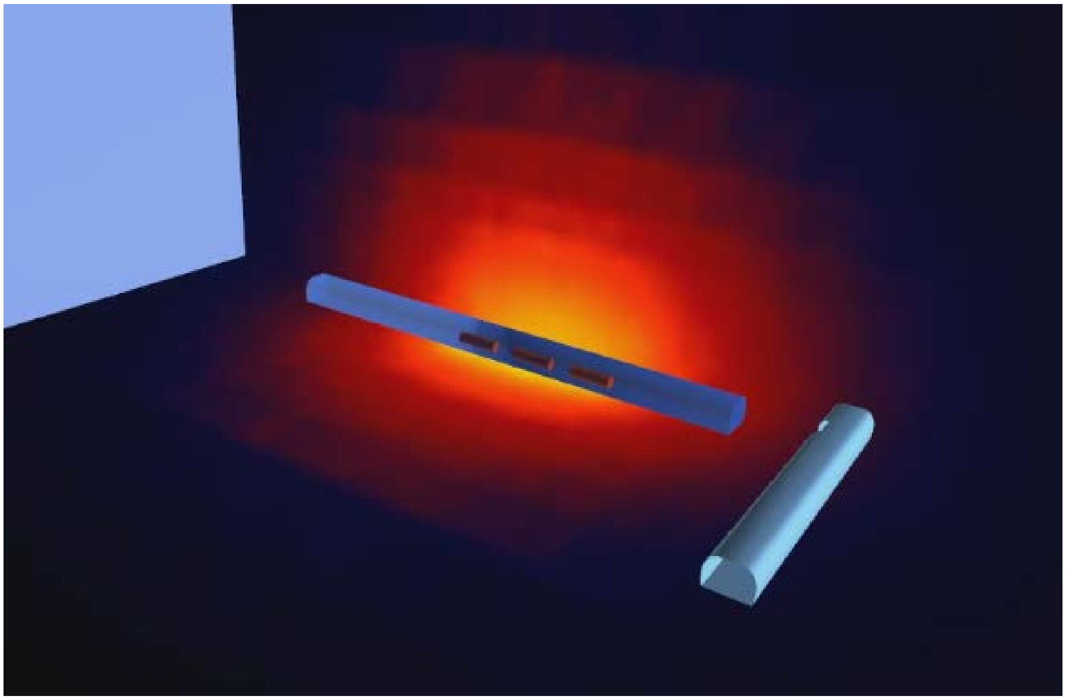

Fig. 6. Calculated temperature distribution around two horizontal heated drifts after 10 years of heating (combined horizontal/vertical section showing one of the heated drifts)

PROSPECTS

Most of the VIRTUS features described in the last sections are already implemented. The proto-typical simulations with the PLC are in preparation. Until early 2014, they will be performed and the entire system will be tested by the project partners.

VIRTUS has been developed, in the current project phase, 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 regarding the VIRTUS functionalities, 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 means will make it a useful tool for all institutions involved in repository research. The implementer can use it for the development and comparison of repository concepts, while research organizations and regulators can use it for evaluation purposes and information of the public.

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