THREE-DIMENSIONAL SIMULATION OF COUPLED GROUNDWATER FLOW AND SALT TRANSPORT IN CONNECTION WITH RADIOACTIVE WASTE REPOSITORIES

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ABSTRACT

Some problems in subsurface hydrology involve coupled groundwater flow and transport of solutes due to changes in the fluid density. Recently, attention has been focused on long-term salt dissolution and brine transport in connection with salt formations that are under consideration as radioactive waste repositories. For salt domes and bedded-salt formations where density variations exceed 20%, the existing numerical codes have emphasized the difficulty of solving strongly coupled flow and transport equations. Numerical simulation capability for flow and transport of strongly coupled variable-density brines is decisive for the performance assessment of such geological formations for isolating radionuclides from the biosphere.

Part of the problems encountered in simulating these sites are related to the nonlinearities of the coupled problem, to the heterogeneous nature of regional aquifers, to the very large finite-element grids needed to avoid numerical instabilities and, to a large extent, also to the very large CPU times needed for three-dimensional simulations. In this paper we briefly review numerical approaches to the coupled problem including recent developed codes and discuss experiences gained from previous modelling studies. We introduce a new, fully three-dimensional, numerical code SoTraCoF developed for treating large problems. Finally, we present an example of the application of the code for a 3D generic model, based on the characteristics of a real site where a regional aquifer overlays a salt dome.

INTRODUCTION

The importance of long-term salt dissolution has been recognized in the scientific community for the quantitative analysis of the long-term safety of underground repositories planned in rock salt. The most extensive quantification possible of the problems related to the disposal of radioactive wastes is the essential aim of most works related with fluid phases through rocks. It is recognized that, the isolation of radioactive material from the biosphere can be influenced by fluid phases through rocks; in this context, salt dissolution may play an important role, positive or negative, in the transport of radionuclides through rocks and into the biosphere. Accounting for all physical and chemical processes related to the underground transport through saltwater-bearing formations, however, is a difficult task because of the strong dependence of fluid density to groundwater velocities.

Numerical models including the complete hydrogeological settings are the most important tools, if not the only, capable of accounting for all geological, hydrogeological and geochemical available information.

Some works have tried to quantify this phenomenon using numerical modelling; among others are: the Konrad site (Rivera et al., 1996), the Morsleben site (Rivera and Ehrminger, 1997), the Gorleben site (Vogel and Schelkes, 1996; Genter et al., 1997), and the Wipp site (Kröhn and Schelkes, 1996). Most of these types of studies have used two-dimensional models; the importance of the third dimension has been recognized, but only a few attempts in the development and/or application to real cases have been successfully completed.

Due to their long-term safety required for waste disposal sites, a complete quantitative analysis requires the solving of problems that are implicitly in four dimensions (3 space dimensions and time); therefore, fully three-dimensional numerical models including times scales are necessary. Building 3-D models, however, is not a trivial task because of the nonlinearities and computer limitations involved, and thus fully 3D conceptual models, as well as advanced and efficient numerical solvers, are needed.

In this work we deal with the subject of developing and applying transient three-dimensional models of coupled groundwater flow and salt transport accounting for variations in fluid density. We attempt to present an overview of the state-of-the-art of numerical modelling for the simulation of groundwater systems including density effects.

We briefly review numerical approaches to the coupled problem including recently developed codes and discuss experiences gained from previous modelling studies. We introduce a new, fully three-dimensional, numerical code SoTraCoF (Genter, 1997) developed for treating large problems. Finally, we present an example of the application of the code for a 3D generic model, based on the characteristics of the Gorleben site.

PRIOR WORK CONCERNING NUMERICAL APPROACHES TO VARIABLE DENSITY FLOW AND TRANSPORT MODELLING

Groundwater density may vary as a result of either concentration or temperature variations. In concentrated brine pools, the fluid density can alter considerably, e.g. to values higher than 1200 kg/m^3. Density differences can introduce gravitational instabilities that may strongly influence the groundwater dynamics. Concentrated salt solutions occur near salt domes (e.g. Gorleben and Morsleben sites, Germany), in deep crystalline rocks (e.g. La Vienne site, France, and the Äspo site, Sweden), and above bedded-salt formations (e.g. Konrad site, Germany, and the Wipp site, USA).

In the past, various codes have been developed to simulate groundwater systems including density effects. In Table 1, we present a summary of a few of the most important of these codes that have been documented, verified, and a few, applied to realistic cases. We don't discuss here those codes that use the freshwater/saltwater interface approach, only those that are fully or partially coupled and that include advection, mechanical dispersion and molecular diffusion.

As can be seen from Table 1, some of these commercial codes are short in their capacities, either they are only one- and two-dimensional or they are not fully coupled, or they differ on their numerical approaches and time dimensions. Although most of them have been verified against well known benchmarks (Elder, salt dome), only a few of them have been applied (and published) to realistic cases where they can show their full capacities.

All the existing commercial codes for solving coupled variable-density groundwater flow and salt transport have advantages and disadvantages; it is difficult to say which one is the best, for their performance strongly depend on their application to a particular problem. For example, some problems can be solved with a partially coupled solution, or in some cases, a two-dimensional model may be sufficient.

Table 1 Codes for variable-density groundwater flow and salt transport

Code name	Dimensions	Coupling	Numerical approach	Time dimension	Verification	References
FEFLOW	2D, 3D	partially	volume fraction	transient	Elder, salt dome	Diersch (1994)
NAMMU	1D, 2D, 3D	fully	mass fraction	steady state and transient	Salt dome, Henry case	Herbert et al. (1988)
ROCKFLOW	1D, 2D	partially	mass fraction	transient	Elder, salt dome	Kröhn (1991)
SoTraCoF	1D, 2D, 3D	partially	volume fraction	transient	Elder, salt dome	Genter (1997)
SUTRA	2D	fully	mass fraction	transient	Elder, Salt dome	Voss (1984)
TOUGH2	2D	fully	mass fraction	transient	Elder, salt dome, Henry case	Oldenburg and Pruess (1995)

According to Table 1, only FEFLOW, NAMMU, SoTraCoF are able to model fully three-dimensional problems. The type of coupling, on the other hand, may be significant if large changes in fluid density are expected; while the numerical approach indicates the code level of the approximation for the balance equations, e.g., if the advective flux is larger than the diffusive/dispersive flux, the volume fraction formulation is sufficient. A few codes (FEFLOW, SoTraCoF) use the extended Boussinesq approximation (Diersch, 1994; Genter, 1998) in the balance equation of the fluid mass, which is very similar to the full density approximation in all balance equations. Of the codes listed in Table 1, only NAMMU is able to solve directly in steady-state. This fact is an indication of the extreme difficulties of numerical solvers to provide direct steady-state solutions for this highly nonlinear problem (Herbert et al., 1988). However, of the listed codes, it is NAMMU the most difficult to apply, the one that uses the largest CPU and demands the most of core space. Additionally, a large level of experience is required to implement it. Thus, although it is probably the most complete and robust of the listed codes, it is not the most efficient in its direct and prompt application.

The reader is referred to Kolditz et al. (1998) who recently published a complete and very elegant discussion of numerical approximations to the balance equations for solute mass and fluid flow used in several codes.

EXPERIENCE FROM PREVIOUS MODELLING STUDIES

Our experience in applying these type of models to realistic field problems, has thought us that the selection of a given code should be based more on its "practical use", that is, on its adaptability, readability and efficiency. It goes without saying that it must had been verified and validated. It should be noted that, to a large extent, the quality of a modelling study of the type discussed here is determined by the efficiency of the model itself on the one hand, and on the expertise of the modelling team on the other hand.

Because of the strongly coupling and the nonlinearities found in the simulation of groundwater flow and salt transport, the development and application of these type of codes has created a field of its own, both in the research environment as well as in the field of their application to site-specific problems. The application of a generic model to site-specific conditions should follow a well-structured model application protocol. The discussion of such protocols is beyond the scope of this paper (see Van der Heijde et al., 1988; Anderson and Woessner, 1992). In the field of radioactive waste repositories, quality assurance applies at all levels of modelling, and, for this type of studies it consists of using appropriate data, data analysis procedures, state-of-the-art modelling methodology and technology, administrative procedures, and auditing.

The main problems found when applying these models to real cases are: grid convergence, heterogeneity of regional aquifers/aquitards, numerical instabilities, large CPU times (in the case of 3D problems), and difficulties to solve for direct steady-state solutions.

When modelling this phenomenon on two-dimensional models, we have observed that because of the contact of rock salt formations with moving groundwater, the otherwise freshwater flow field is strongly affected where it transports and dilutes salt. The consequences are (see for example Wollrath, 1995): the fluid density increases and the fluid pressure increases; the fluid fluxes' magnitude and direction are modified, that is, the groundwater velocities decrease; in some cases there is an onset of recirculation and water becomes stagnant, or it takes dramatically longer times to reach the biosphere; the particle pathways are modified as compared with freshwater simulations; and a "barrier effect" is established (i.e., the reduction of upward flow velocity due to the presence of salt increases the timescale for advective transport of radioactive isotopes).

Thus, the overall results obtained with these modelling studies are positive from the perspective of performance assessment. The net effect that results, in the presence of salt near radwaste sites, is a positive effect on the long-term safety of the proposed sites.

A NEWLY DEVELOPED FULLY 3D CODE: SOTRACOF

Recently, a new numerical code of the type discussed before, was developed in particular for dealing with large three-dimensional models in connection with the study of radioactive waste sites (Genter, 1998). Because its prompt application to a site-specific case, the code has followed the protocol defined above. The current status (SoTraCoF 3.0) includes: new and very efficient modelling methodologies and technology, verification against well known benchmarks (Elder problem, salt dome and Henry case, Genter, 1998) and intercode comparison, and application to two real cases in three dimensions using appropriate data from the Gorleben site in Germany (Rivera et al, 1997) and La Vienne site in France (Rivera and Schindler, 1997).

In this section, we briefly summarize the main governing equations for variable density groundwater flow and solute transport used in SoTraCoF, which are described in detail in Genter (1998).

The fluid mass balance equation is:

$$S_0 \frac{\partial h}{\partial t} + \frac{\partial q_i}{\partial x_i} = Q_h + Q_{EB}(C) \quad \text{..} (1)$$

The solute mass balance equation is:

$$\Phi \frac{\partial C}{\partial t} + q_1 \frac{\partial C}{\partial x_i} - \frac{\partial}{\partial x_i}\left(D_{if} \frac{\partial C}{\partial x_j} \right) = Q_c \quad \text{...................................} (2)$$

Groundwater velocities are obtained from a modified version of darcy's law as:

$$q_1 = -K_{if}\left(\frac{\partial h}{\partial x_j} \right) + \frac{r(C) - r_0}{r_0} e_j \quad \text{...} (3)$$

The coefficient of hydrodynamic dispersion is defined as the sum of mechanical dispersion and molecular diffusion as:

$$D_{ij} = \Phi D_d d_{if} + a_T V_q d_{ij} + (aL - aT)\frac{q_i q_j}{V_q} \quad \text{..........................(4)}$$

The fluid density varies as a function of concentration as:

$$r(C) = r_0 + \frac{\partial r}{\partial C}(C - C_0) \quad \text{..(5)}$$

Finally, the Boussinesq term, Q_{EB} in (1), is defined as:

$$Q_{EB}(C) = -\left(f\frac{\partial r}{\partial C}\frac{\partial C}{\partial t} + \frac{\partial r}{\partial C}\frac{\partial}{\partial x_i} q_i \right) \quad \text{...................................(6)}$$

In these equations h is the hydraulic head, q is the darcy velocity, S_o is the specific storage coefficient, Q_h is a sink/source term for the head and Q_c is a sink/source term for the concentration, Q_{EB} is the extended Boussinesq term, ϕ is the porosity, C is the relative concentration, D is the hydrodynamic dispersion tensor, D_d is the molecular diffusion coefficient, α_L and α_T are the longitudinal and transversal dispersion lengths, respectively, V is the transport velocity, and ρ is the fluid density.

A 3D SIMPLIFIED MODEL BASED ON THE GORLEBEN SITE CHARACTERISTICS

An attempt to simulate this phenomenon with a fully three-dimensional and site-specific model, based on the Gorleben site, has been recently undertaken (Rivera et al., 1997). Although this study is not yet completed, we present a brief description of the work of building the model and simulating the three-dimensional coupled groundwater movement and salt transport with the code SoTraCoF. Our goal here is not to discuss the results of this study but rather to illustrate some practical aspects of this, otherwise difficult, three-dimensional simulation of a realistic application. Because results of this type of work in three dimensions are rare, we want to share the findings of this fundamental type of modelling study. In taking this task, we were aware of the intrinsic limitations: currently available computer resources (hardware), available numerical codes (software), and the complexity of the hydrogeological system (multilayer, heterogenous aquifer/aquitard system).

The site, known as “The Gorleben Salt Dome”, is located in the northeastern part of Germany in the rural Lower-Saxonian district near the river Elbe (Figure 1). The site has been explored since 1979 with regard to its suitability for disposal of all types of solid and solidified radioactive wastes. A very extensive set of data has been collected from hydrogeological investigations through the drilling of about 300 boreholes (BfS, 1990).

An area of about 350 km^2 was first studied with a three-dimensional freshwater model using a very fine finite-element grid (Genter et al., 1997). This first 3D model was used to calibrate the main aquifers of the site and to characterize the freshwater-dominated part of the groundwater system.

Because of potential restrictions on available software and hardware, it was decided to first built a generic and simplified model based on the characteristics of the Gorleben Salt Dome site. The aim of this modelling study was to gain experience in simulating fully coupled groundwater flow and salt transport at the regional scale of a real site in three dimensions, as well as to study the variable-density spatial distribution and its influence on the groundwater movement and transport. Therefore, we followed a step-by-step procedure as described below.

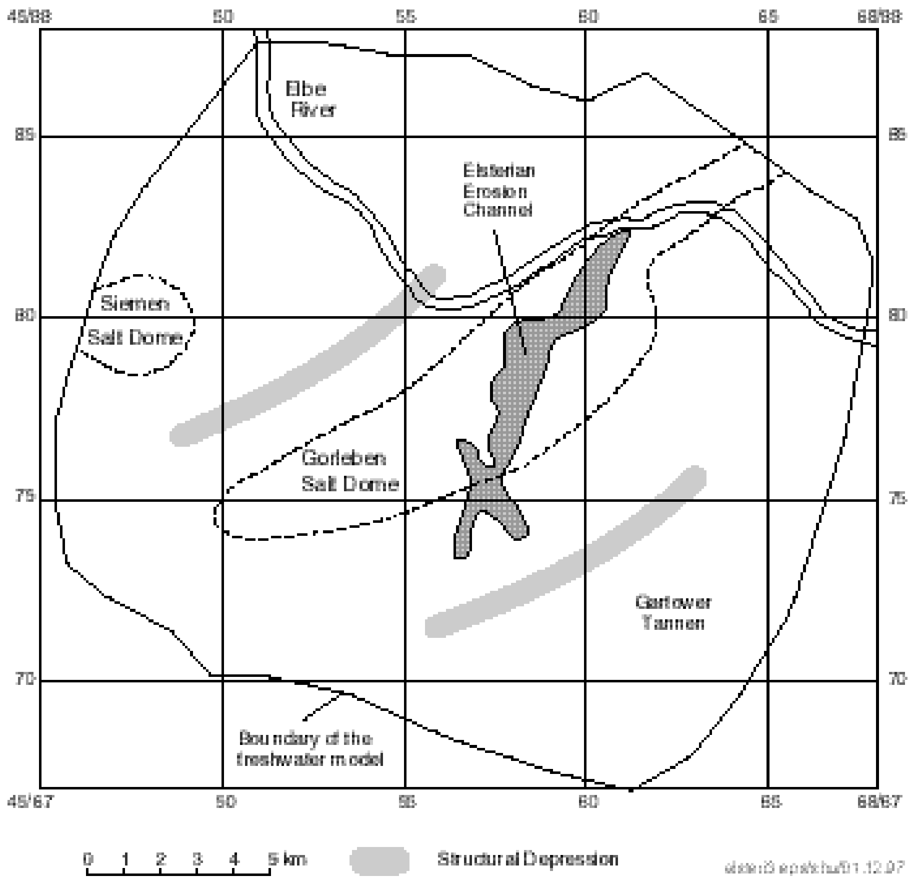

Figure 1 Study area in northeastern Germany.

The extension of this modelling study was reduced to an area of approximately 36 km^2 as compared to the 3D freshwater model. The procedure followed was to begin with a restricted area that included most of the salt dome (shaded area A in Fig. 2), to run the numerical model and evaluate the available software/hardware efficiency, to test various numerical approaches, to evaluate the costs of a long-term transient simulation, and to discern on the importance of the third dimension. After several adjustments and the experienced gained with this first model, it was then decided to extend it further to the west and northwest as shown in Figure 2 (shaded area B) for a total area of about 105 km^2 (A+B in Fig. 2).

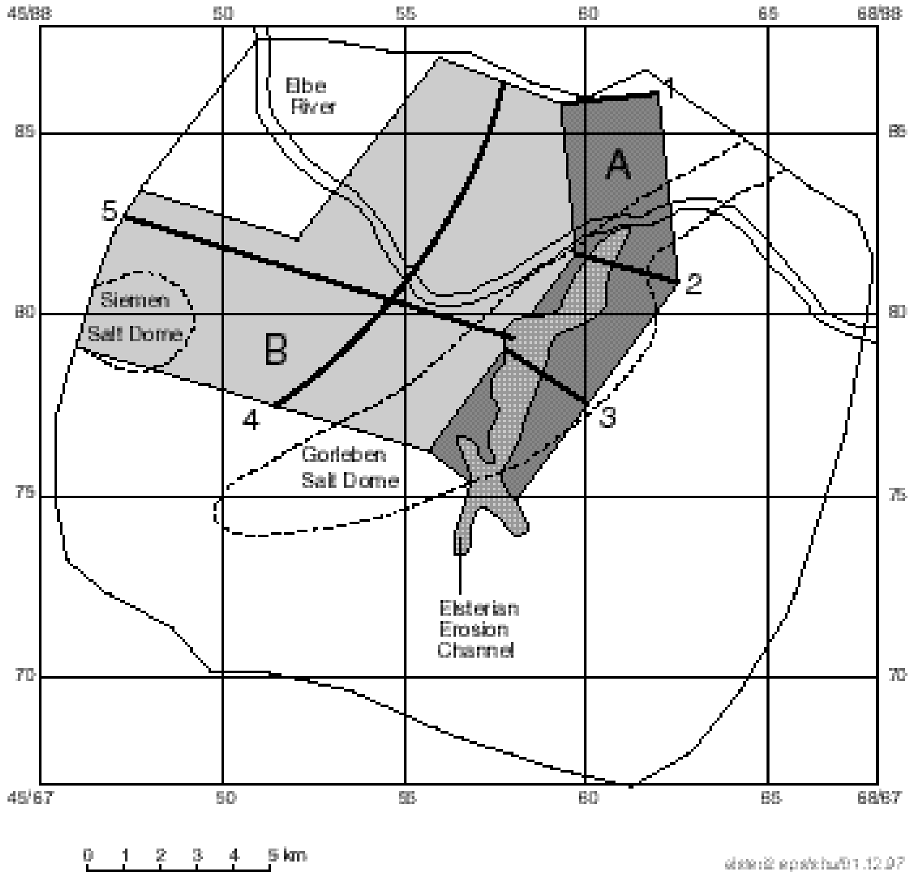

Figure 2 Surface covered by the three-dimensional model.

The 32 hydrogeological units of the original and complete freshwater model were simplified and reduced to 6 hydrogeological units in this coupled groundwater flow-salt transport model. Figure 3 shows some 2D vertical sections through the 3D model (locations are indicated in Figure 2). The sections shown indicate the hydro-geological units considered as aquifers and aquitards in the model, as well as the hydraulic conductivities of each unit. As can be seen, up to 5 orders-of-magnitude differences can be found between some units. The salt dome is included by prescribing a boundary condition of maximum salt concentration at the bottom of the model in an area of about 3 quarters of the surface (from south to north) indicated by the shaded area A in Fig 2.

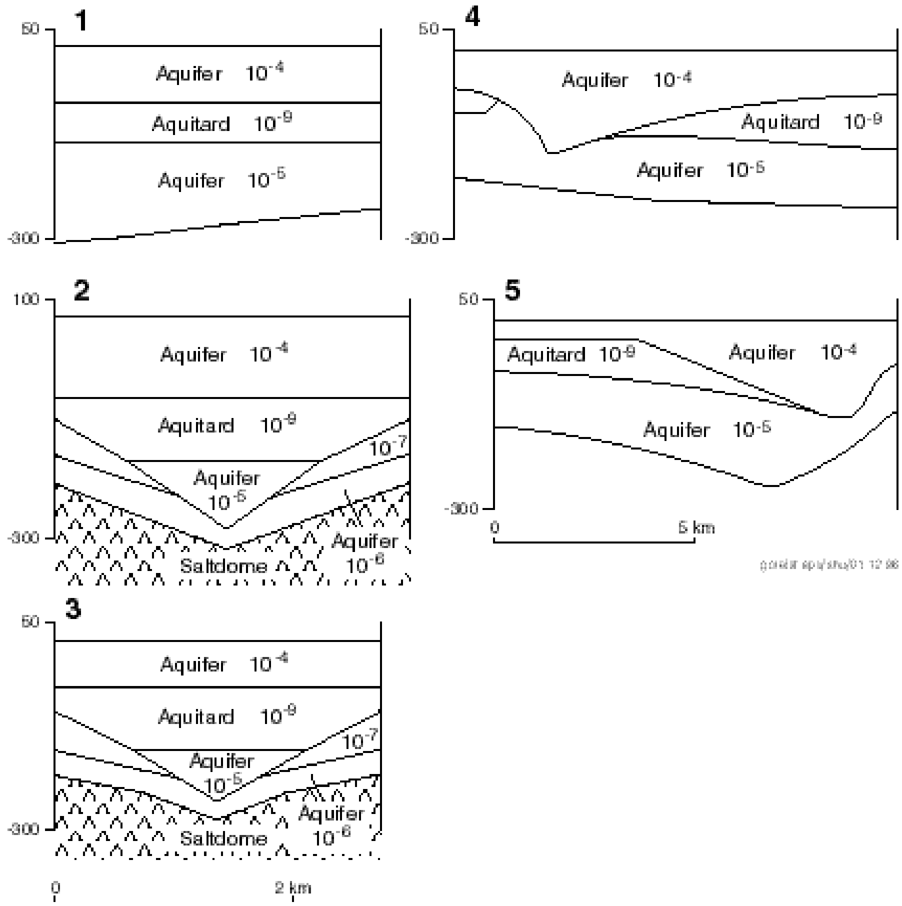

Figure 3 2D vertical sections through the 3D model.

Several convergence tests were first performed in order to design an optimal grid and to reduce numerical dispersion; these tests included various grids with increasing refinements on strategic parts of the model. Next, the code SoTraCoF itself was adjusted in accordance with the numerical model, in particular, this included the search of optimal time-stepping schemes and the testing of various preconditioning methods for the numerical solver.

The other parameters used to run this model (the hydraulic conductivities are indicated in Fig. 3) are: 50 m and 0.5 m for the longitudinal and transverse dispersivities, respectively; $1x10^{-9}$ m^2/s for the molecular diffusion coefficient; a porosity of 20% for all layers with the exception of the lowermost aquifer which is in direct contact with the salt dome (5%); and 10^{-5} m^{-1} for the specific storage coefficient (10^{-6} m^{-1} for the lowermost aquifer). The maximum prescribed salt concentration at the bottom of the model is 297 g/l with a corresponding fluid density of 1200 kg/m^3.

The full 3D model (A + B areas in Fig. 2) is composed of about 106'000 finite elements and about 460'000 nodes. A detailed quantification of the hardware needs for this problem was accomplished by carefully designing the simulation runs and simulated times, based on the available computers. The model was run on a DEC AlphaServer 4100 workstation having 4 processors and 1GB of memory.

Because it was suspected that the local groundwater flow system and salt dissolution is currently in a long-term transient state, we first planned a relatively “short” transient simulation of 20'000 yr to learn about the software-hardware capabilities. A much longer transient simulation (10^5 to 10^6 years) would follow after re-designing and evaluating the costs and efficiency of the overall project.

Table 2 summarises the results of this first set of simulations. It can be noticed that although the model A+B is about 2.5 times larger than model A, the CPU time needed for the same amount of simulated time was relatively shorter; this was due to the adjustment of the time-stepping scheme in SoTraCoF after the analysis of the results from the first model. From this modelling study it became clear that, a middle-term analysis with a fully 3D coupled model takes an enlarged numerical effort and represents a large time-consuming task. While the simulations with 2D models are normally done in the orders of some hours of CPU, a 3D model can take days, or even weeks of runtime on a current workstation, as was learned with this study. On the other hand, if the simulation involves a long-term transient analysis, on the orders of hundreds of thousands of years, then it can take months of runtime.

Table 2 Summary of the results of three-dimensional simulations

Model	Dimensions	Memory	CPU	Simulated time
A	42'366 elements 177'246 nodes	ca. 109 MB	ca. 2 min per time step. Timestep size: 1 to 2 yr	20'000 yr = 15 days of CPU time
A+B	105'350 elements 456'187 nodes	ca. 221 MB	ca. 3.3 min per time step. Time-step size between 200 days and 3 yr	20'000 yr = 30 days of CPU time

Partial and preliminary results are shown in Figures 4 and 5; they show the three-dimensional distribution of the 10% salt concentration after 10'000 and 20'000 yrs, respectively. The dissolution of the salt coming into the system at the contact with the salt dome is done mostly by advective transport along the middle aquifer and some diffusion through the upper aquitard. The salt transport is first directed on a SW-NE axis, it then changes abruptly to the west direction related to the topography of the aquifer basis. Careful analysis of these preliminary results also confirmed the importance of the third dimension when comparing with previous 2D modelling results. The presence of salt in the main central aquifer does not only come from direct upward movement through the lowermost aquifer, which is in direct contact with the salt dome, but it also comes from lateral input from the lowermost aquifer on both sides of the bounding aquitards.

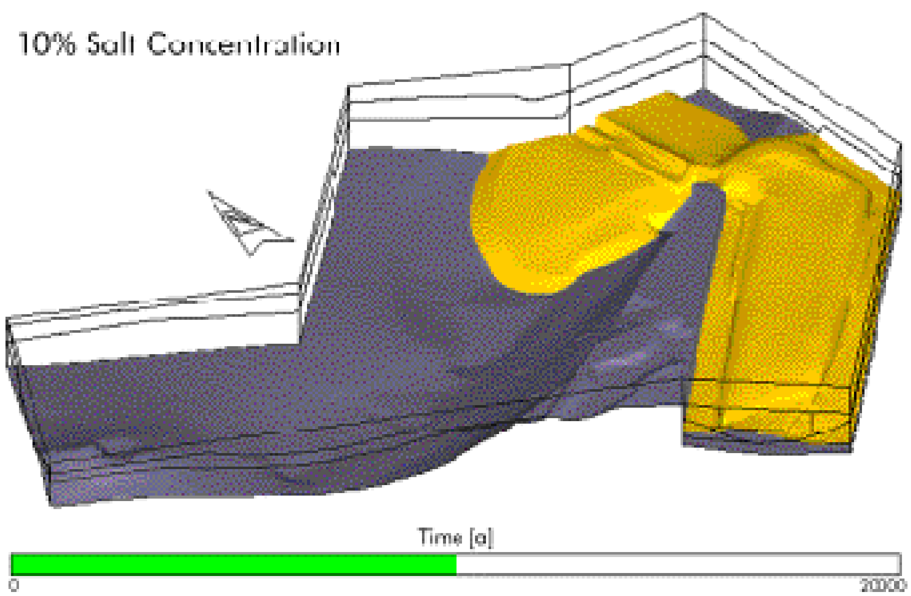

Figure 4 Three-dimensional distribution of 10% salt concentration after 10'000 yr.

Further analysis of this modelling study was performed on the basis of a long-term simulation (e.g., 10^5 a, or more) which was still going on at the time of the preparation of this paper.

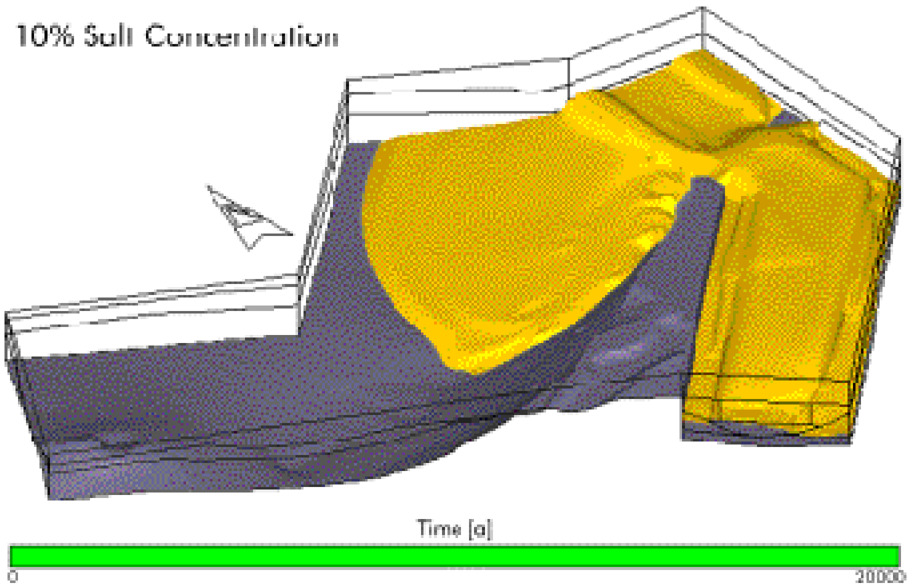

Figure 5 Three-dimensional distribution of 10% salt concentration after 20'000 yr.

CONCLUDING REMARKS

An important step was accomplished in developing and testing a three-dimensional variable- density numerical model, as well as to applying it to a realistic, although simplified and generic, site-specific model. The simulation of coupled groundwater flow and salt transport in the context of radioactive waste repositories has proven to be a large time-consuming task with an enlarged numerical effort. However, the experience on practical aspects gained with this numerical study is very rich and may be useful for carefully designing other similar studies. Final conclusions concerning this particular study can still not be accomplished, for the results analysed in this paper are only partial. A similar procedure as the one described here, is currently being applied to other three-dimensional problems (La Vienne site; Rivera and Schindler, 1997).

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KEY WORDS

Groundwater modelling, SoTraCoF, three-dimensional simulation, salt transport, radioactive waste.