MODELLING DENSITY-DRIVEN FLOW USING d³f

A. SCHNEIDER✉ and E. FEIN

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH.
Theodor-Heuss-Str. 4, D-38122 Braunschweig, Germany
E-mails: scn@grs.de, fei@grs.de

Abstract

d³f (distributed density driven flow) is a software package for the modelling of density-driven groundwater flow especially in large, three-dimensional, and hydrogeologically complex domains with up to several millions of nodes. It is suited for modelling of coastal problems as well as for groundwater movement in the vicinity of salt domes.

The first test case is the groundwater flow model in the overburden of the salt dome of Hoefer in Lower Saxony, Germany. The model consists of four layers, two thereof are aquifers. The influence of the salt dome is represented by a Dirichlet boundary condition for the concentration. Simulations are carried out with up to one million of nodes and over a model time of 10 000 years.

A second application is the overburden of the Waste Isolation Pilot Plant (WIPP), a repository for transuranic waste in New-Mexico, USA. Both two and three-dimensional models consisting of six layers were developed. The WIPP-Site model can be regarded as an extreme test case because it contains two extremely thin sheets and permeabilities varying about eight orders of magnitude. Simulations are carried out using up to 250 000 nodes over a model time of 20 000 years.

Keywords: software code, groundwater, density-driven flow, salt dome, seawater, porous media

Introduction

In Germany salt is regarded as a potential host medium for nuclear waste disposal. To be able to model groundwater flow in the overburden of salt domes over long time periods the software package d³f has been developed. The development has been performed under project management of the GRS on behalf

✉ Corresponding author

of the Federal Ministry of Education, Science, Research and Technology (BMBF) by working groups at six universities from 1995 to 1999 (Fein and Schneider, 1999).

d^3f is suited for the two- and three-dimensional modelling of density-driven groundwater flow through porous media with salt concentrations up to saturation. The permeabilities of the hydrogeological units may vary over several orders of magnitude. The modelling is restricted to confined aquifers.

Advection, diffusion and dispersion are regarded as transport processes. Fluid density and viscosity are functions of salt concentration and temperature. Dispersion is modelled by the Scheidegger's approach. The permeabilities are defined as constants, as functions or stochastically. User-defined functions may be assigned to initial and boundary conditions.

The simulator is based on the software package UG (Unstructured Grids, Bastian *et al.*, 1997). The discretization is performed by means of a finite volume method with a consistent velocity approximation. An upwind-algorithm may be selected. Adaptive grids and time-steps, controlled by a-posteriori error estimators, can be used. A linear multigrid technique combined with a BiCGStab-algorithm is implemented as solver. d^3f can be run on LINUX-pcs, workstations, clusters and massively parallel computers, too. This provides the ability to model large, three-dimensional, and hydrogeologically complex areas with up to several millions of nodes.

The d^3f-package contains interactive, graphical pre- and postprocessors. The preprocessor affords the possibility to create input data files for 3D models starting from digitized hydrogeological cross sections or subsurface contour maps. During the last four years two new 3D grid generators have been developed, one creating hexahedrons (Feuchter *et al.*, 2001) and the other creating tetrahedrons (Fuchs and Wittum, in prep.) and, for selected layers, prisms. This is especially important if the model domain contains extremely thin layers.

d^3f is suited to model coastal problems and freshwater lenses below islands as well as for applications with salt concentrations up to saturation such as groundwater movement in the vicinity of salt domes. To verify the code several 2D and 3D test problems had been modelled and its results had been verified by measuring data (Birthler *et al.*, 2000, Johannsen *et al.*, 2002). The aim of the actual project is the modelling of density driven flow in several realistic, large, 3D domains with complex hydrogeological structures using d^3f (Schneider and Birthler, 2004).

The salt dome of Hoefer, Lower Saxony, Germany

Simulation works are carried out to model groundwater flow in the overburden of the salt dome of Hoefer. It is situated in Lower Saxony, Germany, in the North of Hanover, near the town of Celle. The salt dome is embedded in marly and limy materials, overlaid by Tertiary clays and sands with a thickness up to 300 m. These are overlaid by Quaternary sands containing loamy-clayey layers.

The model extends over a length of 7 km, a width of 5 km and a depth of 150 m. It consists of four layers, two aquifers, one clay layer and the deeper, Tertiary beds that are composed to one layer referred to as

Tertiary (see Figure 1). The upper aquifer doesn't cover completely the modelled domain. On the permeabilities, there exists some measured data (Dahms and Neubert, 1984); the other parameters like porosities, diffusion and dispersion lengths were taken from literature. The parameters used are compiled in Table 1.

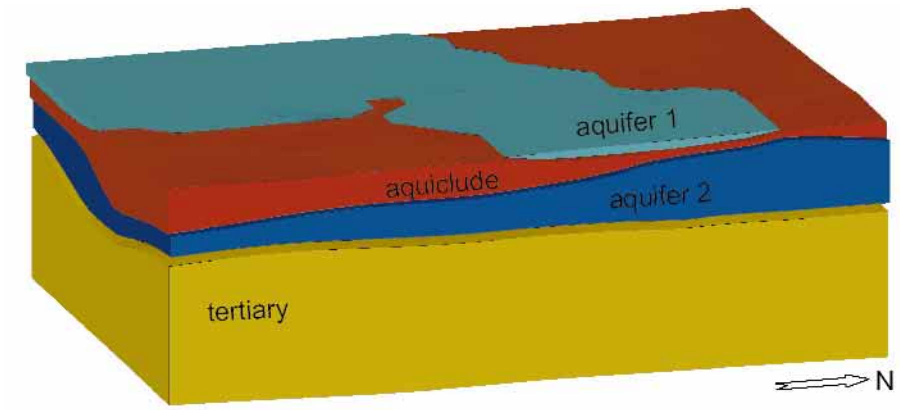

Figure 1. The different layers of the 3D-model of Hoefer.

Table 1. Model parameters of the hydrogeological units.

Unit	k [m^2]	ϕ [-]	D_m [m^2 s^{-1}]	α_L [m^2 s^{-1}]	α_T [m^2 s^{-1}]
first aquifer	$5 \cdot 10^{-11}$	0.35	$1.0 \cdot 10^{-9}$	10.0	1.0
aquiclude	$2 \cdot 10^{-17}$	0.2			
second aquifer	$3 \cdot 10^{-11}$	0.3			
Tertiary	$1 \cdot 10^{-13}$	0.2			

Groundwater density and viscosity are modelled as linear functions of the NaCl concentration. The density varies from 1000 kg m^{-3}, if the concentration is 0.0 kg kg^{-1}, to 1200 kg m^{-3} for saturated brine with a concentration of 0.260 kg kg^{-1}.

The influence of the salt dome is represented by a Dirichlet boundary condition for the concentration (see Figure 2). Here, the variable c represents the relative mass fraction, and c = 1 stands for saturated brine. The bottom of the model area is considered to be impermeable. At the top, the model is limited by the groundwater level (Hoffmann, 1981) and consequently a Dirichlet boundary condition for the pressure is used. Concentration is set to zero. On the lateral boundaries hydrostatical pressure conditions are used and the concentration is assumed to be zero, too. As initial condition, the model domain is completely filled with freshwater, and a hydrostatical pressure distribution is assumed.

A coarse grid consisting of tetrahedrons with 2,478 nodes was created. Simulations were carried out with up to one million of nodes and over a model time of 10,000 years, until a quasi-steady-state was reached. The differences in the hydraulic-heads induce a diagonal flow across the model area from the northeast to the southwest. The steady-state velocity field is depicted in Figure 3.

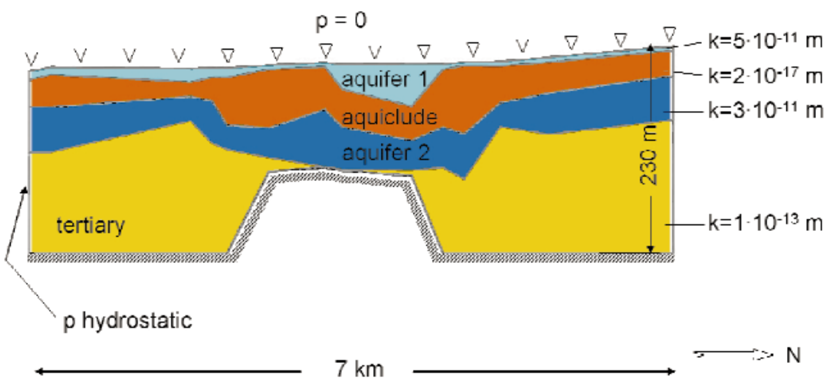

Figure 2. Vertical cross section of the 3D Hoefer model

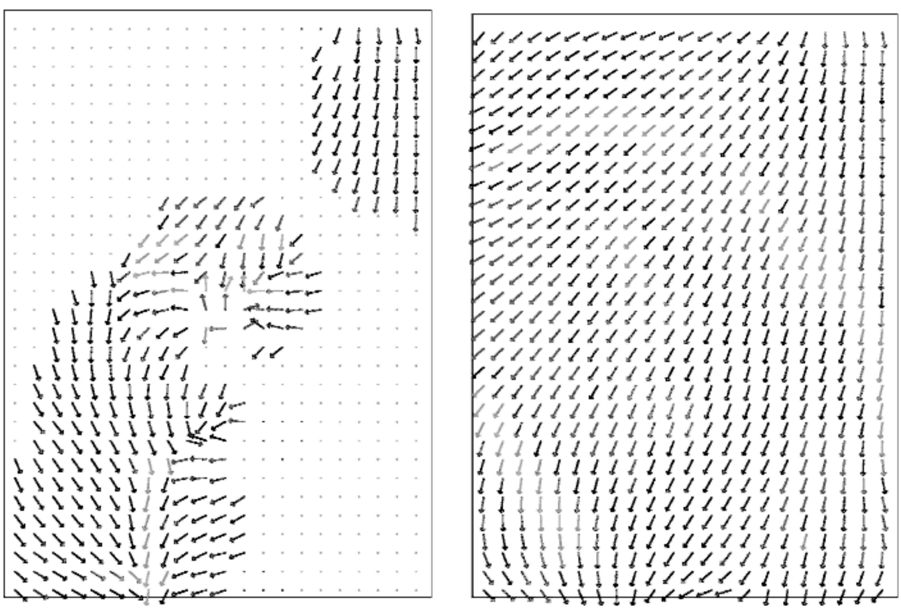

Figure 3. Stationary velocity field of the Hoefer model: aquifer 1 (left), aquifer 2 (right).

The salt plume mainly spreads into the mainstream direction up to the second aquifer. The concentrations on a diagonal cutting plane from the northeast to the southwest are shown in Figure 4. Only a minor part moves into the opposed horizontal direction to the bottom of the domain, caused by the higher density of saline waters. Hence a convection cell arises in the northwest of the salt dome (see Figure 5).

Reaching the second aquifer the saline waters become highly diluted because of the flow velocity which is three orders of magnitude higher than in the Tertiary sediments. So the water quality in both aquifers remains below the limit for potable water of about $c = 0.002$.

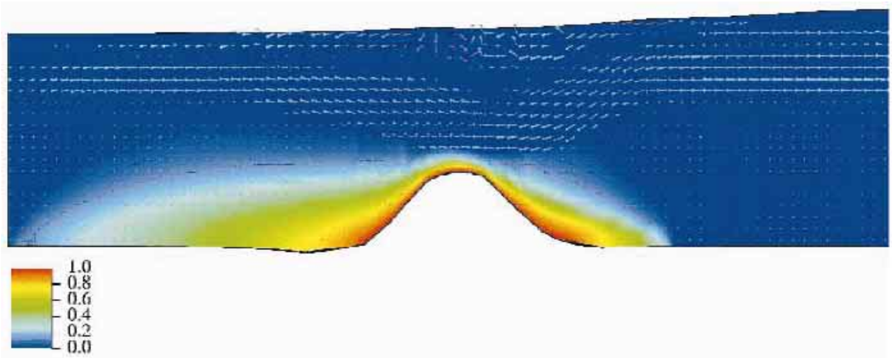

Figure 4. Stationary concentration and velocity field of the Hoefer model.

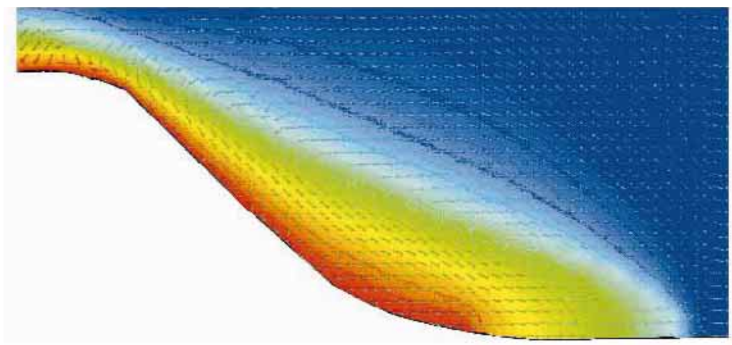

Figure 5. Convection cell arising in the Hoefer model.

The WIPP-Site, USA

A further application is a 3D modelling of the overburden of the Waste Isolation Pilot Plant (WIPP), a repository for transuranic waste in New-Mexico, USA. It is situated in a hilly terrain declining in a westward direction with height differences of about 300 m. Mountain ranges in the south, north and west form some kind of a basin structure that extends over an area of 30 km x 30 km. The Rio Pecos from the northwest to the southeast forms a receiving watercourse. Eastwardly the Nash Draw is located; a large depression sloped towards the Rio Pecos and a groundwater-fed salt lake.

Geological setting

The WIPP-Site is situated in a semi-arid territory with a groundwater level located at great depth below the surface. The hydrogeology of this site is well explored (DOE, 1986). It is characterised by a flat-lying stratification and extremely thin sheets. NaCl concentrations up to a saturated brine have been measured in groundwater.

The repository is located at a depth of about 660 m b. s. l. within a Zechstein formation which is 500 m thick, the so-called Salado. It consists of halite and includes layers of anhydrite, polyhalite, dolomite and clay. Above of the Salado water-conducting formations exist, which have been modelled within this project: the Rustler formation, the Dewey Lake Red Beds, the Santa Rosa and the Gatuña formations.

The Rustler formation belongs to the Zechstein too, and is divided into five layers, the Unnamed Lower Member, the Culebra Dolomite, the Tamarisk, the Magenta Dolomite and the Forty Niner. The last three of them crop out within the model region, as shown in Figure 6. The properties of the layers differ considerably:

- The Unnamed Lower Member has a thickness of about 36 m and consists of a sequence of silty rock, anhydrite and halite, that changes westward into its solution residue. This formation has a low permeability.
- The highly permeable Culebra Dolomite is only 7.7 m thick and covers the whole region. It contains heterogeneities as cavities and enclosures of other materials. Permeabilities vary from 10^{-17} m^2 in the eastern part to 10^{-11} m^2 in the west.
- The Tamarisk is low permeable and has a thickness of 25 m. It consists of two anhydrite layers that are divided by a halite layer and in the western part by its solution residue, respectively.
- The Magenta Dolomite presents a similar thickness as the Culebra and has one order of magnitude lower permeability.
- The Forty Niner is the top layer of the Rustler formation and is similar to the Tamarisk formation.
- The Dewey Lake Red Beds mainly consist of low permeable clay, silt and sandstone with vertical, gypsum-filled fractures and has a thickness up to 150 m in the east. It is covered by the Dockum Group and some Quaternary layers of low thickness that are of minor importance for the hydrogeological model. There exists measured data for permeabilities and porosities (Davies, 1989).

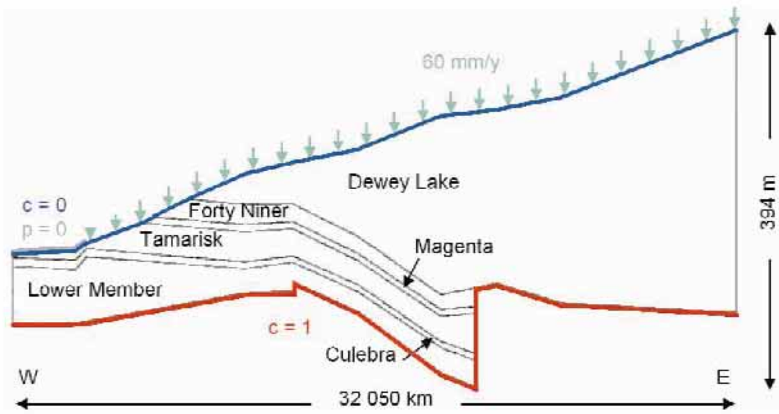

Figure 6. Vertical cross section of the WIPP-Site model.

Hydrogeological model

Due to the high permeability of the Culebra Dolomite, and because of restrictions in computer capacities, recent models only focused to the Culebra formation and presumed impermeability of all other layers. Later, chemical analyses (Chapman, 1988) and models (Corbet, 1992; Davies, 1989) led to another concept, and hence the contributions of the low permeable layers to groundwater dynamics are taken into account, too. Here a hydraulically closed groundwater system is supposed confined by the mountain ranges, which are regarded as watersheds, and by the Rio Pecos.

Following these assumptions in the early 1990s, within the international INTRAVAL-project, a 2D model has been developed based on a vertical cross-section that extends from the mountain ranges to the Nash Draw (Schelkes *et al.*, 1995). The location of this cross-section is shown in Fig 7. The model has a length of 32 km and a depth of about 400 m. It contains the Rustler, the Dewey Lake Red Beds, the Santa Rosa and the Gatuña formations.

Since the Dockum Group and the Quaternary layers are of less importance for groundwater movement, they are combined with the Dewey Lake Red Beds to one layer named Dewey Lake. The Salado is assumed to form the impermeable bottom boundary of the model. The top of the model is defined by the surface level. This model serves as the basis for both the 2D and 3D model in this project.

Numerical model

Firstly a 2D model was constructed. It consists of six layers as shown in Figure 6. The cross–section is indicated in Figure 7. The parameters are specified corresponding to Schelkes *et al.*, (1995), see Table 2. Permeabilities are assumed to increase linearly from east to west.

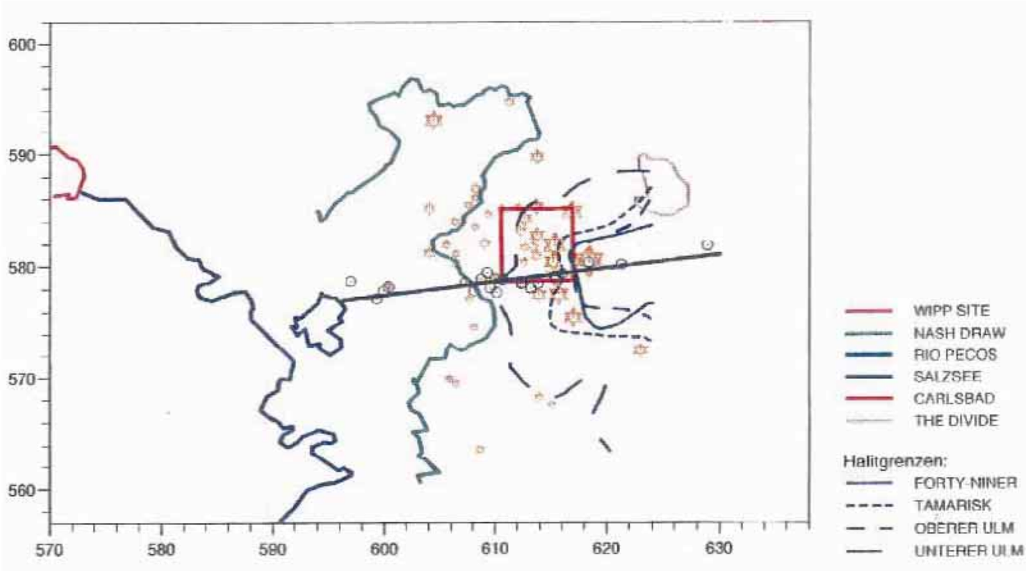

Figure 7. WIPP-Site: Position of the vertical cross section (Schelkes *et al.*, 1995).
✡ Density measurement points in the Culebra Dolomite formation.
○ Boreholes.

Salt is dissolved from the Salado formation and additionally from the halite strata in the eastern part of the Rustler formation. To be able to model these salinity conditions as boundary conditions the saline, mainly impermeable parts, are not included in the model. So the bottom boundary is provided with the Dirichlet-condition $c = 1$ for saturated brine. Bottom and lateral boundaries are assumed to be impermeable.

At the top boundary an inflow velocity corresponding to a groundwater recharge of 60 mm/y is given except for a small, lower part in the west where a Dirichlet-condition $p = 0$ is defined. The concentration is set to zero.

Groundwater density and viscosity are modelled in the same way as described above. In the initial state, the model is completely filled with freshwater, and the pressure is distributed hydrostatically.

In Schelkes *et al*. (1995) the permeability contrasts between neighbouring layers are weakened by the introduction of artificial additional layers in between. Here the full contrasts are modelled.

The 2D model is meshed by a triangle grid. The coarse grid consists of 6,169 nodes, see Figure 8. Simulations were performed with a two-grid-algorithm with 23,034 nodes and again with three grids and 88,855 nodes.

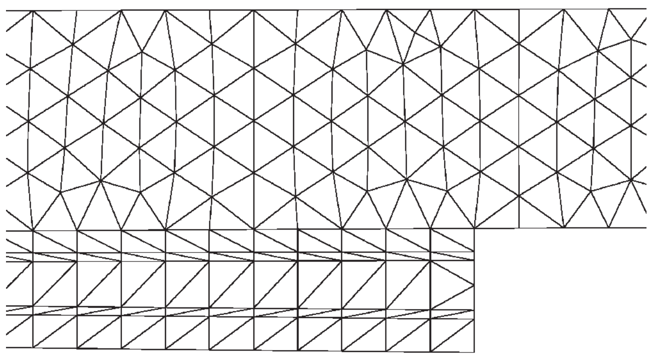

Figure 8. Cut-out of the 2D grid of the WIPP model.

Table 2. Model-parameters of the hydrogeological units.

Unit	k [m^2]	ϕ [-]	D_m [$m^2\ s^{-1}$]	α_L [$m^2\ s^{-1}$]	α_T [$m^2\ s^{-1}$]
Dewey Lake	$1\cdot10^{-15}$	0.15	$1.0\cdot10^{-9}$	10.0	1.0
Forty Niner	$1\cdot10^{-19}$ to $1\cdot10^{-13}$	0.14			
Magenta	$3\cdot10^{-18}$ to $1\cdot10^{-12}$	0.14			
Tamarisk	$1\cdot10^{-19}$ to $1\cdot10^{-14}$	0.14			
Culebra	$3\cdot10^{17}$ to $1\cdot10^{11}$	0.15			
Lower Member	$1\cdot10^{-19}$ to $3\cdot10^{-14}$	0.10			

The 3D model was built by the prolongation of the 2D cross-section into the third direction over a length of 10 km. A hexahedron grid with 693 nodes was created (see Figure 9). Simulations were performed on three grid levels with 32,439 nodes and on four levels with 245,245 nodes.

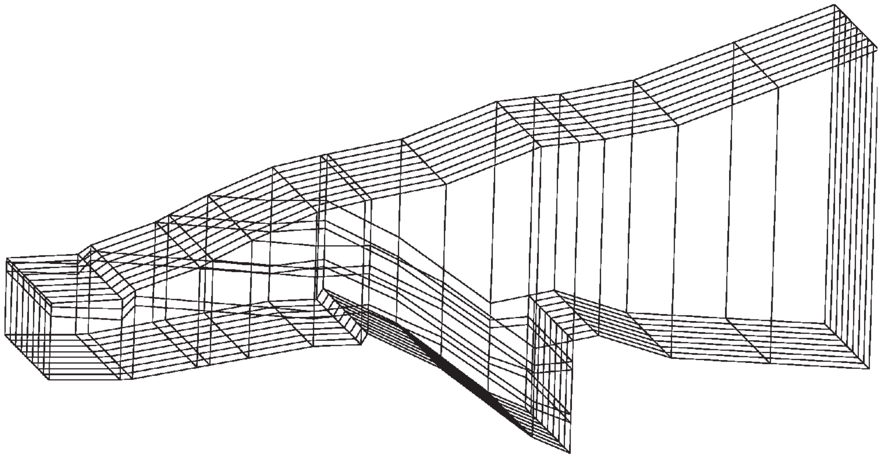

Figure 9. 3D grid of the WIPP-Site model.

Results

All results presented were obtained sequentially on LINUX-workstations. The steady state was reached after a model time of about 20,000 years. The two-dimensional calculations needed 31 and 35 time steps and a computational time of 60 and 100 minutes, respectively, to reach steady state.

The simulated, stationary concentration distributions show only very small differences in the western part of the model. In the velocity field no differences are visible (see Figure 10 and Figure 11). One can see that the main transport of saline waters takes place within the Culebra Dolomite, where the highest velocities occur with $3 \cdot 10^{-6}$ m s^{-1}.

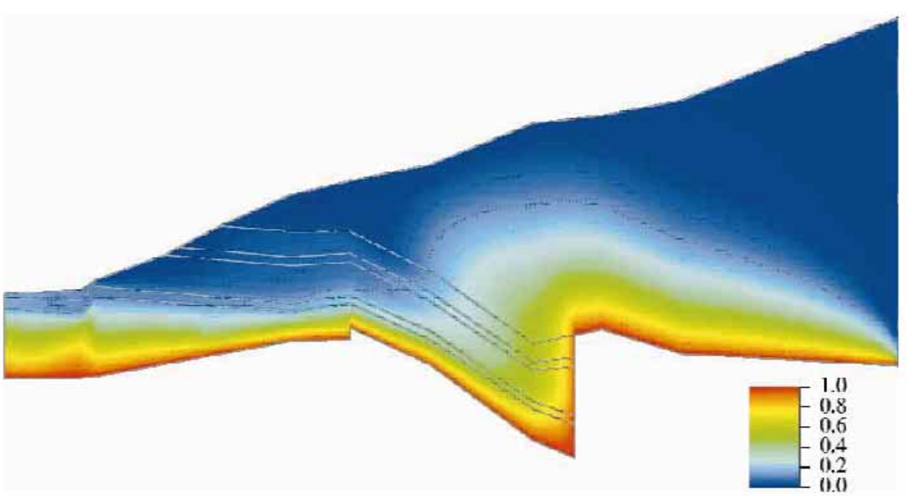

Figure 10. Steady-state concentration of the 2D WIPP model (vertically exaggerated by a factor of 40).

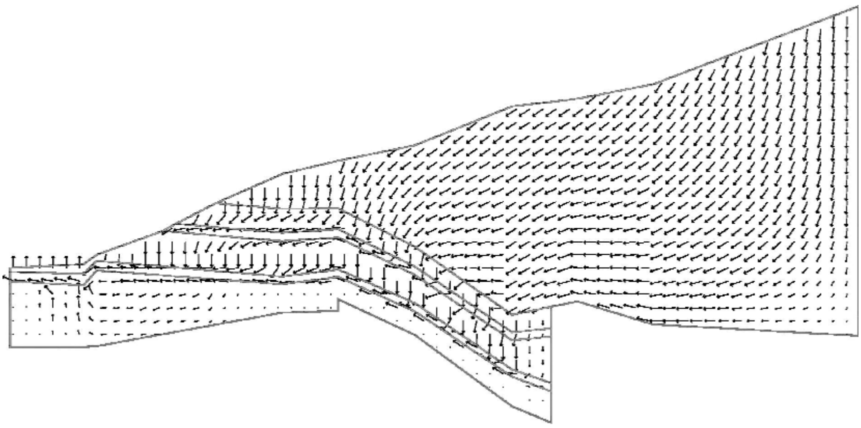

Figure 11. Steady-state velocity field of the WIPP model (vertically exaggerated, vectors scaled by 1000)

The 3D simulations were calculated on hexahedron grids. A problem is the very small thickness of the Culebra Dolomite of 7.7 m. This is confronted with horizontal element lengths of some thousands of meters. The worst aspect ratio amounts about 1:550. This, together with the permeability differences of the Culebra Dolomite to its neighbouring layers of up to eight orders of magnitude, implies an extremely bad quality of the computational matrix.

The 3D simulation on 32,439 nodes reached the model time of 20,000 years after 54 time steps and 110 minutes on a LINUX-workstation. The simulation with 245,245 nodes reached a model time of 3,500 years after 16 weeks computing time.

The simulated concentrations show differences only in the eastern part, where the grid elements are especially large. Differences in the velocity fields are not observable. The 2D and the 3D simulations show the same results.

Of the fluid density in the Culebra Dolomite there exists a lot of measurement data (Davies, 1989). These are used for a validation of the model results (see Figure 12). The results of Schelkes *et al.*, (1995) largely correspond to the measured values. It is remarkable that all 2D and 3D d³f simulations show exactly the same results, but these results show small discrepancies to the measured data. This may be caused by the difference in the models, the neglect of the eastern parts of the Rustler-layers.

In the case of the 3D WIPP model, it was only possible to perform sequential simulations during this project. But since that time the parallel solvers were improved by the d³f developers at the University of Heidelberg, so that it is now possible to run simulations with much finer grids on parallel computers, too.

Conclusions

Two realistic 3D test-cases are modelled with the software package d³f. The first application is the simulation of groundwater flow in the overburden of the salt-dome of Hoefer in Lower Saxony, Germany.

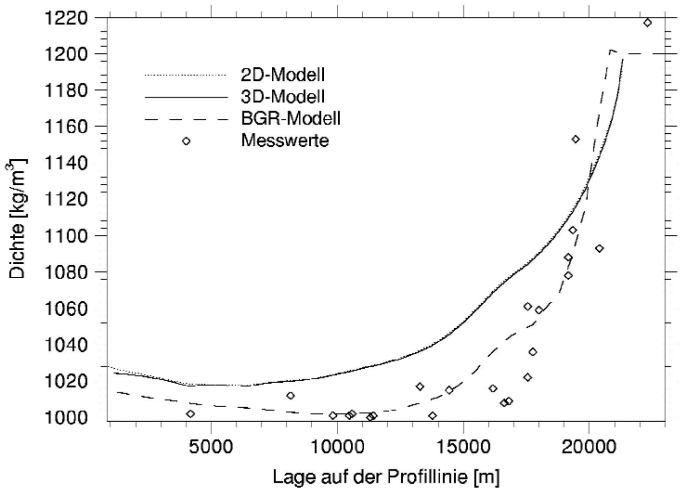

Figure 12. Comparison of measured and calculated fluid density in the Culebra Dolomite formation.

The model consists of four layers, two aquifers and two aquitards. Computations are carried out over a model time of 10 000 years. This test case shows that d^3f is able to model density-driven flow with salt concentrations up to saturation in large, three-dimensional, realistic domains with up to one million of nodes.

The second model is the Waste Isolation Pilot Plant (WIPP), a repository for transuranic waste in New-Mexico, USA. Both two- and three-dimensional models were developed. The models consist of six layers. The main aquifer has a thickness of about 7.7 m and a permeability that is about eight orders of magnitude higher as in the neighbouring layers. Simulations are carried out over a model time of about 20,000 years and using up to 250,000 nodes. The results show only small discrepancies to measurement data. This application demonstrates that d^3f is suited for the modelling of density-driven flow in large, hydrogeologically complex domains with extremely thin layers and with high permeability contrasts.

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