Density-driven flow modelling using d³f

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ABSTRACT

The finite volume code d³f (distributed density driven flow) has been developed with a view to modelling large, complex, density-influenced aquifer systems. The use of cutting-edge numerical methods and their parallelisation enables simulations over long time periods with feasible computational effort. Developed for long-term safety analyses for nuclear waste repositories, d³f is applied here to a series of laboratory experiments regarding fresh water lenses of islands, as well as to a coastal aquifer near the German North Sea (work in progress.)

INTRODUCTION

The code d³f (distributed density driven flow) has been developed to meet the needs of far field modelling as a part of long-term safety analyses for nuclear waste repositories in rock salt. It is able to model density-driven flow in the overburden of salt domes, i.e. in areas up to 10 000 km² with complex hydrogeological situations over time periods of some ten thousands of years. The development began in 1995 as a joint project of GRS together with five university institutes, funded by BMWi, and is still ongoing. The result is a powerful tool that is able to handle salt and heat transport in porous as well as fractured media, salt concentrations up to saturation and complex hydrogeological structures with high permeability contrasts. Besides safety analyses, d³f has been applied to other fields, too, such as laboratory and field experiments or coastal aquifers.

THE MODEL

The finite volume code d³f is based on the UG toolbox, uses fast numerical solvers such as multigrid methods and is completely parallelized (Fein 1999). Currently, d³f solves the following equation system describing thermo-haline flow:

$$\partial_t(\phi\rho)+\nabla\cdot(\rho\mathbf{q})=0 \qquad (1)$$

$$\partial_t(\phi\omega\rho)+\nabla\cdot(\rho\omega\mathbf{q}+\mathbf{J}_\omega)=0 \qquad (2)$$

$$\mathbf{J}_\omega=-\rho\mathbf{D}\nabla\omega, \quad \mathbf{D}=D_m\boldsymbol{\tau}+\mathbf{D_d} \qquad (3)$$

$$\partial_t\left[\left(\phi\rho C_f+(1-\phi)\rho_s C_s\right)T\right]+\nabla\cdot(\rho C_f T\mathbf{q}+\mathbf{J}_T)=0 \qquad (4)$$

$$\mathbf{J}_T=-\boldsymbol{\Lambda}\nabla T \qquad (5)$$

$$\mathbf{q}=-\frac{k}{\mu}(\nabla p-\rho\mathbf{g}) \qquad (6)$$

where (1) describes the mass conservation of the fluid, (2) the mass conservation of the brine, (3) diffusive/dispersive flow, (4) energy conservation, (5) heat flow and (6) Darcy's law. Hereby, ϕ is the porosity [-], ω the solute mass fraction [-], $\rho(\omega)$ the fluid density [kg m^{-3}], t the time [s], $\mathbf{q}$ the Darcy velocity [m s^{-1}], k the permeability [m^2], $\mu(\omega)$ the dynamic viscosity [Pa s], p the pressure [N m^{-2}] and $\mathbf{g}$ the gravitation vector [m s^{-2}]. D_m represents the molecular diffusion constant, $\boldsymbol{\tau}$ the tortuosity tensor, and $\mathbf{D_d}$ the dispersion tensor [m^2 s^{-1}] according to Scheidegger's law (Bear 1972). C_f is the specific heat capacity of the fluid [J kg^{-1}K^{-1}], C_s the specific heat capacity of the solid (rock) [J kg^{-1}K^{-1}], ρ_s the rock density [kg m^{-3}], T the temperature [K] and $\boldsymbol{\Lambda}$ the hydrodynamic thermal dispersion tensor [m^2 s^{-1}]. The fluid density ρ and the dynamic viscosity μ are depending on salt mass fraction and temperature. It should be mentioned that the complete equations for flow and salt transport are solved without simplifications such as the Boussinesq approximation. The application of d^{3}f is restricted to saturated conditions. A free groundwater surface is represented by means of a level set method. For detailed description see Fein (1999), Schneider (2012).

RESULTS

Reported here is the modelling of a couple of quasi-2d laboratory experiments performed by BGR to investigate the dynamics of freshwater lenses. Hereby, an acrylic sand box with a size of 2 m x 0.3 m x 0.05 m was used to simulate formation and degradation of freshwater lenses. Based on the experimental results a benchmark was defined, consisting of the lens formation by applying, and lens degradation after stopping recharge. For a description of the experiments and parameters in detail see Stoeckl (2012) and (2014). The benchmark was simulated numerically by five computer codes. Thereby, all codes had to use the same computational grid as well as the same numerical parameters. In the first step, a very coarse grid was used, consisting of 7380 nodes. Regarding concentration, d^{3}f results fitted very well with FEFLOW results, see figure 1. Remarkable was the very thin transition zone between fresh- and saltwater that was calculated by d^{3}f in spite of the prescribed coarse discretization.

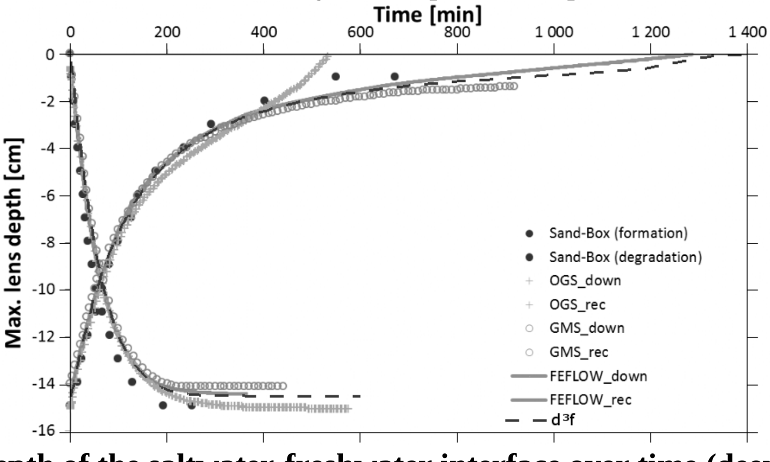

Figure 1: Depth of the saltwater-freshwater interface over time (deepest point) – comparison of the results of OpenGeosys, Seawat (GMS), FEFLOW and d^{3}f with the measurements (source: preliminary results after L. Stoeckl, modified)

In a second step the simulations were repeated on a finer grid consisting of 121 362 nodes (results see Stoeckl 2014). Because d^{3}f numerics are based on multigrid methods, we performed additional simulations on a multigrid from 1 617 to 394 497 nodes. Furthermore, the sensitivity to various factors was investigated, such as solving the full equation system in comparison to using the Boussinesq approximation, the influence of different variations of boundary conditions and the level of grid refinement.

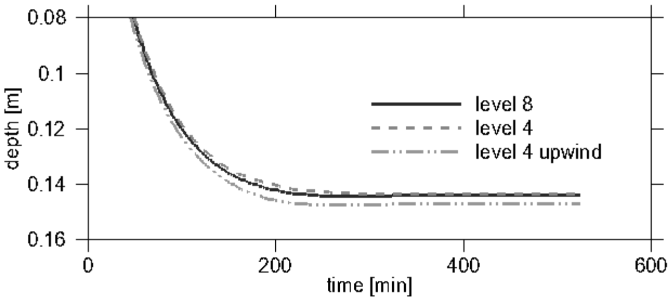

Figure 2: Depth of the saltwater-freshwater interface over time
results on 394 497 (level 8) and 1 617 nodes (level 4) as well as using upwind methods

The results on the 121 362 nodes grid and on multigrid level 8, 7 and 6 almost completely coincide. Using Boussinesq approximation had also no observable influence. Figure 2 shows the relatively low influence of the grid refinement on the depth of the lens, whereas using upwind methods on relatively coarse grids may distort the result significantly. In figure 3 is illustrated, that the transition zone and especially the width of the outflow zone may easily be overestimated without an appropriate grid refinement or using upwind methods.

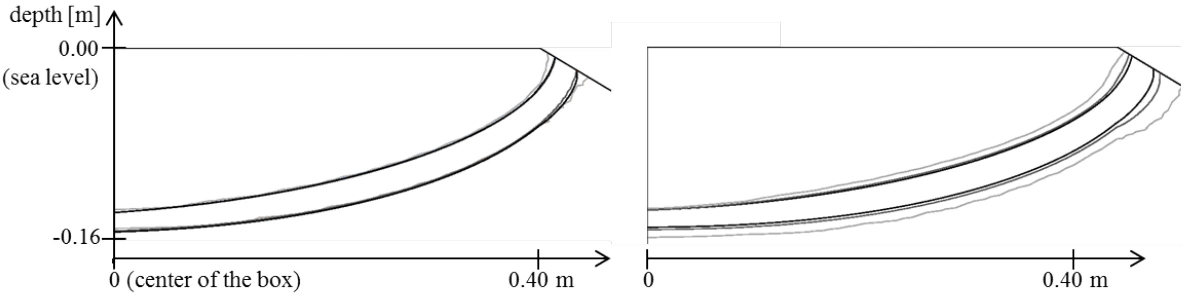

Figure 3: Thickness of the saltwater-freshwater transition zone
isolines of 10 % (upper lines) and 90 % concentration, results on grid level 8 (black line), 6 (grey line) and 4 (light grey line); left: without upwind, right: with upwind method

Additionally, some variations of the experiment were simulated as well, such as changes in recharge and the introduction of less permeable zones in horizontal as well as in vertical direction (Dose et al. 2013.) Here, only one example is shown, where the left part of the sand box was filled with a more than 10 times lower permeable material ($k = 2.15 \cdot 10^{-10}$ m²) than the right ($k = 2.35 \cdot 10^{-9}$ m²). This inhomogeneity strongly influences the shape of the freshwater lens and the situation of the watershed. After reaching steady-state the lens is much deeper in the left hand part, and a change in its slope at the boundary between the two permeability sectors is clearly visible in the results (see Figure 4). The results of d^{3}f and FEFLOW are almost identical. The experimental results could also be reproduced satisfactorily, except for the fact that both numerical codes overestimated the extension of the outflow zone on the higher permeable side.

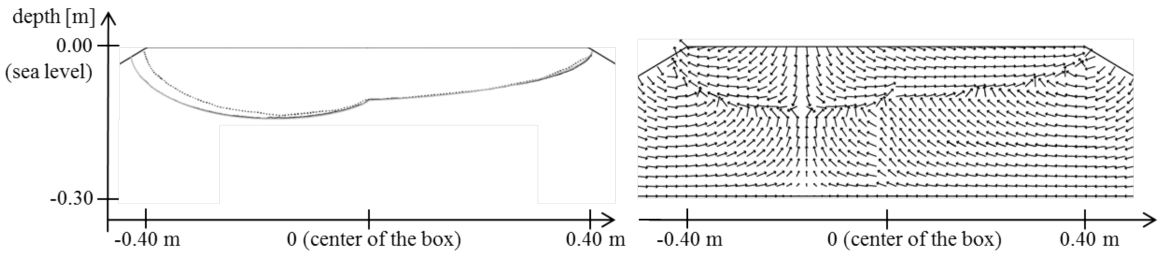

Figure 4: **Left: Depth of the freshwater lens (50 % seawater concentration)**
grey line: d^{3}f, black line: FEFLOW, dotted line: measurements; Right: velocity vectors (d^{3}f)

In an ongoing project, d³f is applied to coastal aquifers near the German North Sea. The aim of this works is forecasting the impact of different climatic and demographic scenarios on the freshwater supply (see also Eley et al 2014). A regional 3d density-driven flow model will be set up, including pumping wells of three waterworks. Scenarios to be simulated are sea-level elevation as a consequence of climate change, shifts of the seasonal distribution of precipitation and changes in the fresh water demand caused by demographic and economic factors.

For now, a 2d vertical cross-section is extracted and adapted for d³f. Simulations are started with the objective of getting acquainted with the hydraulic processes in the model domain as well as testing the interaction of the various features and instruments. First results will be presented here.

CONCLUSIONS

It is shown that the density-driven flow code d³f is applicable to saltwater intrusion problems in laboratory and field scale.

For this type of problem solving the complete set of equations has no advantage over using the Boussinesq approximation because only low salt concentrations are involved. However one has to be very careful in using numerical parameters as grid refinement and upwind methods.

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