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A three-dimensional physical model for verification of variable-density flow codes

S. E. OSWALD

Colenco Power Engineering Ltd, Mellingerstrasse 207, CH-5405 Baden, Switzerland
e-mail: sascha.oswald@colenco.ch

W. KINZELBACH

Institute of Hydromechanics and Water Resources Management, Swiss Federal Institute of Technology, HIL G 37.3, CH-8093 Zurich-Hoenggerberg, Switzerland

Abstract Flow and transport in saturated porous media are influenced or even dominated by the effects of density flow if solute concentration gradients are high. The numerical codes used in the simulation of these nonlinear phenomena have to be tested in order to ensure their reliability. A series of laboratory experiments with well-defined experimental parameters for two typical variable-density flow problems were performed to obtain the data required for benchmarking. A Nuclear Magnetic Resonance Imaging technique was used to measure the three-dimensional salt concentration distribution in a porous medium, including its time evolution. The first problem studied was an unstable density layering of denser saltwater above less dense freshwater, and the onset of finger instabilities was observed. The second case was a stable layering of saltwater below freshwater influenced by discharge of water at the top and resulting in a time-dependent upconing. Numerical simulations of the problems were performed with three different variable-density flow codes and compared with the experimental results.

INTRODUCTION

Variable-density flow in porous media can be caused by differences in temperature and/or concentration. What significance these differences have concerning the actual flow situation also depends on permeabilities, flow and boundary conditions, as well as on the time scale. This study focused on cases of concentration differences only.

Examples of practical problems involving density flow include seawater intrusion in coastal regions, groundwater flow around geological salt formations, intrusion of ancient saltwater in freshwater aquifers and sinking of plumes originating from landfills.

VERIFICATION OF VARIABLE-DENSITY FLOW CODES

Modelling of groundwater flow is important for an improved understanding and the prediction of solute transport processes. In cases of complex flow phenomena, such as variable-density flow, the codes used for modelling have to be verified in some way before their results can be accepted.

The verification of a numerical model of variable-density flow can be viewed in various ways. It can involve the verification of the mathematical functioning of the code or the verification of the adequacy of the model equations used. The mathematical functioning of a code can be tested by analytical solutions or constructed exact solutions (e.g. Schwarz, 1999). A benchmark based on the comparison of numerical with experimental results includes inseparable use of both types.

The benchmarking tests widely used for variable-density codes are: the Henry problem of seawater intrusion comparing numerical results with the known semi-analytical solution (e.g. Segol, 1994; Oswald *et al.*, 1996); the Hydrocoin problem (Level 1, Case 5) of a simplified salt dome (OECD, 1988); and the Elder problem of fingering in a non-stable situation (Elder, 1967). These benchmark tests are all two-dimensional and they are either not sensitive or the solution is not really known exactly but the problems have become customary for the intercomparison of codes.

Field studies can hardly be used as benchmarks for codes. The limiting factors usually are parameter uncertainty due to the poor accessibility of spatial information in aquifers, and the heterogeneity of natural porous media. By using tracer tests between boreholes it is possible to get some information but this information is of an integrative nature.

However, in the laboratory, spatial flow and concentration data are much more easily accessible than in the field. Therefore, laboratory studies are better suited for the verification of numerical models and for investigations into many basic concepts. Experimental conditions are well controlled and characteristic properties can be chosen in advance to meet the conceptual assumptions to a high degree. Hence, there are an increasing number of two-dimensional laboratory experiments suited for comparison with numerical results, e.g. Schincariol & Schwartz (1990), Oostrom *et al.* (1992), Wooding *et al.* (1997).

METHODS

Magnetic Resonance Imaging procedure

The technique of Magnetic Resonance Imaging (MRI) represents a measurement method capable of non-invasive data acquisition on flow and transport at high resolution on a three-dimensional domain. This method was used to visualize tracer transport, using contrast agents as a tracer, to determine time-dependent concentration distributions in a box filled with a porous medium (e.g. Greiner *et al.*, 1997). Copper sulphate ($CuSO_4$) was added to the saltwater as a paramagnetic tracer. Concentrations were chosen low enough to get a linear signal-to-concentration relation. The MRI was performed in slices of 4–5 mm thickness with an image plane resolution of 2.3 mm using a spin-echo imaging sequence (Oswald *et al.*, 1997).

The experiments were carried out on a 1.5 Tesla wholebody MRI system (Magnetom SP 63/84, Siemens or Gyroscan ACS/NT, Philips) built for medical purposes. MR images were acquired from up to 50 adjacent slices before and during the experiments. The tracer behaviour was observed over a period of up to 3 h with a temporal resolution of about 3 min.

Experiments

In the first type of experiments the flow pattern induced by an unstable layering of saltwater above freshwater was observed. In this particular case no external flow was applied and the flow was entirely driven by density effects. A cubic container with 0.24 m side length was filled with silica glass beads (average diameter 0.5 mm) and a cuboid zone with larger glass beads (average diameter 1.2 mm) was inserted into the centre. The extensions of this zone were 40 mm in the two horizontal directions and 160 mm in the vertical direction. Its permeability was calculated from the Kozeny-Carman equation to 1.0×10^{-9} m^2 which was about five times higher than the permeability of the surrounding medium. The permeability ratio was decreased to about three in a second experiment by increasing the size of the beads in the surrounding outer part to 0.7 mm average diameter.

The salt solution of 0.3% salt mass fraction introduced in the upper part of the saturated packing contained mainly NaCl and the paramagnetic tracer $CuSO_4$ at a concentration of 6 mmol l^{-1}. For these low concentrations the driving forces for flow, and hence flow velocities, are small enough to make 3-D imaging possible. The convection process was started by cautiously removing the plastic sheet, which initially separated the denser, saltwater from the freshwater below. An advective fingering of saltwater and freshwater occurred from the beginning simultaneously with mixing by diffusion and local dispersion. The fingering started first in the zone of higher permeability where the degree of instability, as for example expressed by a Rayleigh number, is largest. Then fingers also developed in the zone of lower permeability. The saltwater fingers in the centre coalesce and pool when reaching the end of the zone of higher permeability (Fig. 1).

The second series of experiments was performed for the case of a stable layering of saltwater below freshwater. The setup was similar to the one used in the fingering experiment, but the inner length of the cubic container was 0.2 m. The homogeneous filling consisted of glass beads with a diameter of 1.2 mm. In additional column

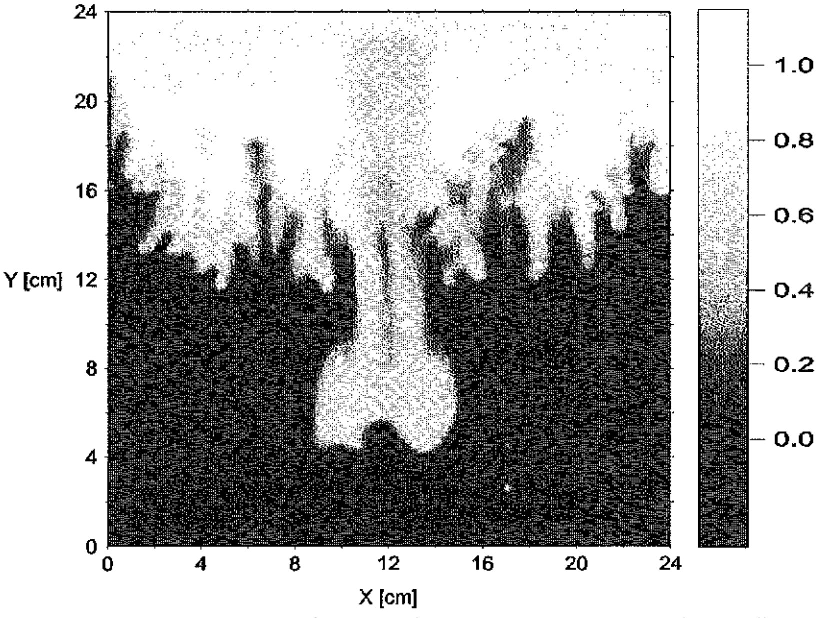

Fig. 1 Vertical cross-section of measured concentrations. White colour indicates maximum concentration, black colour pure freshwater.

experiments the permeability of the porous medium was determined to be 1.0×10^{-9} m^2 and the longitudinal dispersivity to be 1.2 mm.

For MRI two different salt solutions were used which had a total salt concentration of 1.0% salt mass fraction and 10.0% salt mass fraction, respectively. The tracer concentration in both cases was about 10 mmol l^{-1}. An additional recharge–discharge of water at two diagonal corners on the top caused a time-dependent upconing of the saltwater below the abstraction and an outflow of salt in the discharged water. When the density difference between the saltwater and freshwater was increased, the upconing was reduced by gravity forces and the flow pattern changed significantly.

SIMULATIONS

Codes

Simulations of the problems were performed with three different variable-density flow codes and compared with the experimental results: (a) d^{3}f (Fein & Schneider, 1999) based on finite volumes, Newton-Raphson method, adaptive grid, multigrid solver; (b) FEFLOW (Diersch, 1994) based on Galerkin finite elements (FE), extended Boussinesq assumption; (c) SALTFLOW (Frind & Molson, 1994) based on rectangular FE, explicit advection term, Boussinesq approximation. Furthermore, the sensitivity of the numerical results was studied for some of the parameters involved (Oswald, 1998).

Unstable layering

The data obtained in the first experiment were used to test the capabilities of d^{3}f and SALTFLOW. The numerical simulations of the experiments cannot be compared with the experimental MRI data point by point due to the unstable nature of the phenomenon which leads to a non-unique concentration distribution. Therefore, more generic flow properties such as finger growth speed or finger size should be evaluated from experimental and simulated data.

In the simulation the start of the fingers was always delayed compared to the MRI data. This delay is shortened if the numerical grid is refined. The finger growth rate of the experimental data could be reproduced well (Fig. 2). Another simulation including a periodic initial perturbation shortened the delay but reduced the finger growth speed and hence was not capable of simulating the effect of the real perturbations responsible for finger initialization. Numerical stabilization features tended to suppress the onset of fingering. All simulations failed to show the fingering observed in the low permeability area.

Stable layering

The simulation of the second series of experiments starting with an initially stable situation is better suited for benchmarking due to its deterministic behaviour. Besides

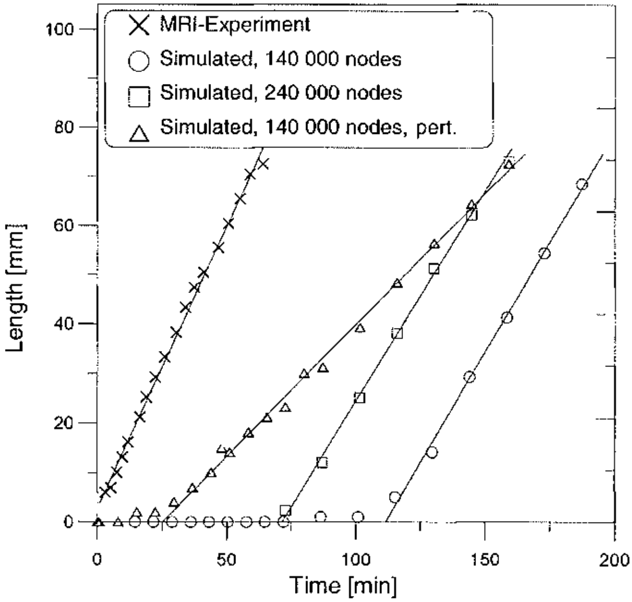

Fig. 2 Measured *vs* simulated finger growth rates in centre of container, "pert." indicating the use of a perturbation of the initial concentration at the interface (calculations with SALTFLOW).

the comparison of the fully three-dimensional isolines at several points in time, one can also compare the cross-sectional concentration isolines. Figure 3 shows, for example, that in the diagonal, vertical cross-section at the end of the experiment with low density contrast, the calculated isolines are already closer to the discharge point at the top than the measured ones. Such differences are probably due to numerical dispersion in the calculations and possibly a small horizontal deviation of the measurements.

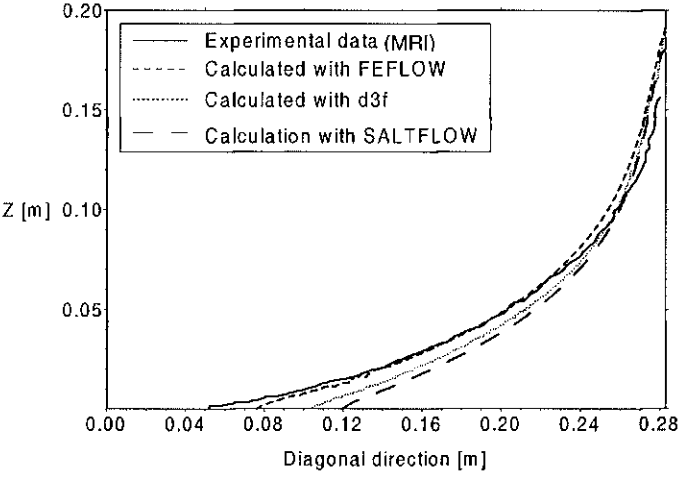

Fig. 3 Vertical cross-section of concentration isolines at the end of the experiment. Inflow at the left top corner, outflow at the right top corner.

A further possibility for comparing the experiments and simulations is independent concentration measurements via electrical conductivity in the discharged water which yields a time-dependent breakthrough curve. In the case of the low density contrast, the simulations reproduced the general shape of the breakthrough curves well, though all show a larger concentration than measured, indicating the presence of numerical dispersion. In the case of the high density contrast the differences between simulated and measured results are larger than before and none of the simulations could reproduce the breakthrough curve properly.

CONCLUSIONS

Two different kinds of variable-density flow situations have been studied. It was possible to evaluate the values of the experimental parameters of these laboratory experiments with high accuracy, and the setup of the problem was quite simple in terms of its geometry and its homogeneity. The experimental results are therefore suitable for the verification of variable-density flow codes. The measurements performed in this work represent new three-dimensional benchmarks which can serve to test the reliability of these codes.

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REFERENCES

Diersch, H.-J. (1994) *FEFLOW User's Manual Version 4.2*. WASY GmbH, Berlin, Germany.

Elder, J.-W. (1967) Transient convection in a porous medium. *J. Fluid Mechanics* **27**(3), 609–623.

Fein, E. & Schneider, A. (1999) *d³f—Ein Programmpaket zur Modellierung von Dichteströmungen*. Abschlussbericht GRS-139, Braunschweig, Germany.

Frind, E. & Molson, J. (1994) *SALTFLOW 2.0 User Guide*. Waterloo Centre for Groundwater Research, Canada.

Greiner, A., Schreiber, W., Brix, G. & Kinzelbach, W. (1997) Magnetic resonance imaging of paramagnetic tracers in porous media: quantification of flow and transport parameters. *Wat. Resour. Res.* **33**(6), 1461–1473.

OECD (1988) The International Hydrocoin Project, Level 1: Code Verification. *OECD, Report no. 71617*. Organisation for Economic Co-operation and Development, Paris, France.

Oostrom, M., Hayworth, J. H., Dane, J. H. & Güven, O. (1992) Behavior of dense aqueous phase leachate plumes in homogeneous porous media. *Wat. Resour. Res.* **28**(8), 2123–2134.

Oswald, S. (1998) Dichteströmungen in porösen Medien: Dreidimensionale Experimente und Modellierung (Variable-density flow in porous media: three-dimensional experiments and modelling). PhD Thesis, ETH Zürich, Switzerland. Dissertation no. 12812.

Oswald, S., Schwarz, C. & Kinzelbach, W. (1996) Benchmarking in numerical modelling of density driven flow. In: *Proc. Fourteenth Saltwater Intrusion Meeting, SWIM 96*, 32–40. Geological Survey of Sweden, Report no. 87.

Oswald, S., Kinzelbach, W., Greiner, A. & Brix, G. (1997) Observation of flow and transport processes in artificial porous media via magnetic resonance imaging in three dimensions. *Geoderma* **80**(3–4), 417–429.

Schincariol, R. A. & Schwartz, F. W. (1990) An experimental investigation of variable density flow and mixing in homogeneous and heterogeneous media. *Wat. Resour. Res.* **26**(10), 2317–2329.

Schwarz, C. (1999) Dichteabhängige Strömungen in homogenen und heterogenen porösen Medien (Density-driven flow in homogeneous and heterogeneous porous media). PhD Thesis, ETH Zürich, Switzerland. Dissertation no. 13028.

Segol, G. (1994) *Classic Groundwater Simulations*. PTR Prentice Hall, Englewood Cliffs, New Jersey, USA.

Wooding, R. A., Tyler, S. W. & White, I. (1997) Convection in groundwater below an evaporating salt lake: onset of instability. *Wat. Resour. Res.* **33**(6), 1199–1218.