Benchmarking in Numerical Modelling of Density Driven Flow

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For the prediction of density driven flow in aquifers one has to rely on numerical codes developed for that purpose. To prove the capability and reliability of these codes benchmark tests are necessary. This study is concerned with benchmarking for density effects due to the influence of salt water, in both two and three dimensions.

Henry's problem

For the problem of seawater intrusion in a coastal aquifer *Henry* (1964) presented a two-dimensional case, for which a semi-analytic steady-state solution exists. Henry's problem has been widely used as a benchmark for density driven flow codes. However, this problem is not sensitive to the performance of transport codes with respect to consistency of velocities and description of small transition zones (*Voss and Souza*, 1987). Recent results and our own calculations show that beyond this deficiency even the utilisation of the Boussinesq approximation and the use of relatively coarse grids do not affect the results significantly. The previously observed differences between model results and the semi-analytic solution of Henry seems to be irrelevant since *Segol* (1994) presented a revised calculation of the semi-analytic solution (Fig. 1a).

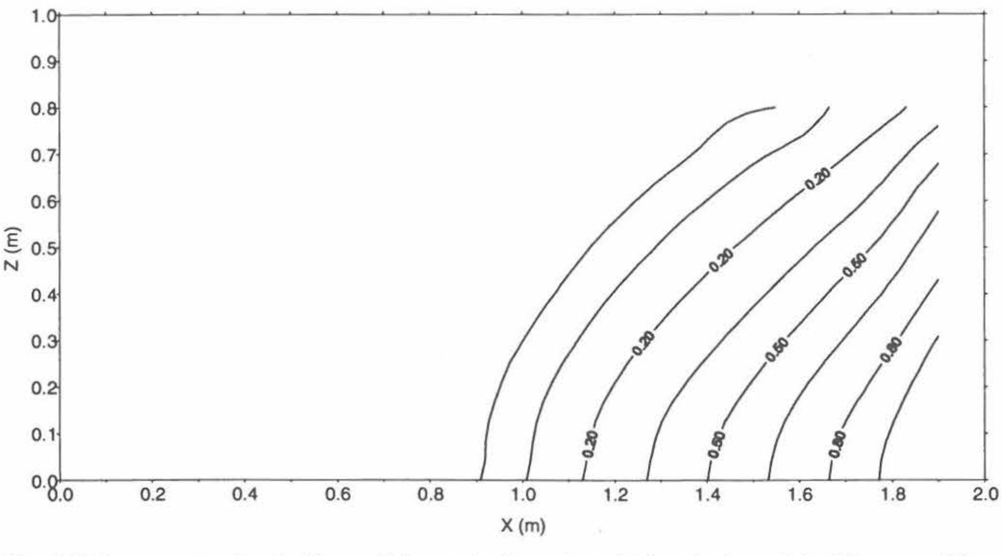

Fig. 1 Salt concentration isolines of the revised semi-analytic solution of the Henry problem (Segol, 1994); inflow from the left, fixed seawater concentration at the right, diffusion coefficient D = 18.86×10^{-6} m^2/s.

In the numerical calculations four different codes were used for comparison purposes:

- FEFLOW (*Diersch*, 1994): Galerkin finite elements (FE), extended Boussinesq approximation
- MARCEAU (*Oltean et al.*, 1994): mixed hybrid FE for flow and dispersion, discontinuous FE for advection
- SALTFLOW (*Frind and Molson*, 1994): rectangular FE, explicit advection term
- ug (*Bastian et al.*, 1995): finite volumes, multigrid solver

The solutions obtained with these codes all match Segol's revised solution very closely, provided the appropriate diffusion coefficient is used. The isochlors evaluated with the four different codes are virtually identical to each other and to the semi-analytic solution (see Fig. 1b). Increasing the resolution of the grid does not change the results any more and also the velocity field, in most cases a more sensitive measure, is not a sensitive indicator of model inaccuracy here. If the seaside boundary conditions for concentrations are modified (in comparison to Henry's problem) to describe a more realistic situation the agreement between the models still prevails.

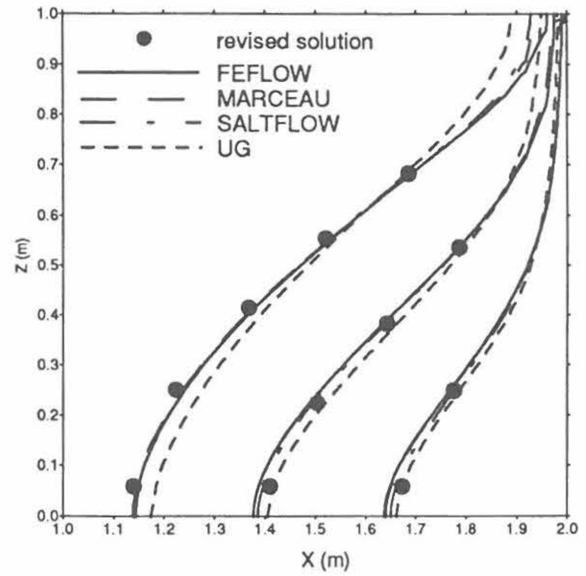

Fig. 1b Comparison of calculated isochlors with the revised solution obtained by Segol (1994). Isochlor values are 20%, 50% and 80% of seawater concentration.

Since the Henry problem can only be used as a benchmark to a very limited extent, more complex, maybe three-dimensional situations of seawater intrusion, have to be considered, i.e. layered or locally heterogeneous aquifers, time-dependent freshwater discharge and/or pumping wells. This types of more realistic problems have been looked into on the field scale, e.g. by *Frind* (1982, 1994), *Huyakorn* (1987) or *Xue* (1995). However, the advantage of having a semi-analytic solution to compare with is lost, and hence one has to use consecutive refinement or comparison with possibly incomplete field data to judge the quality of results. Another widespread benchmark test, the Elder problem (*Elder*, 1967), is indeed more complex due to its unstable nature, but it is only two-dimensional and can only be checked against experimental data of density flow caused by temperature differences.

Miscible density fingering

A second objective of this study is to model saltwater flow driven by density effects on a local scale in a case, in which the results of numerical modelling can be compared to well-controlled laboratory experiments. The physical phenomenon studied is the development of saltwater fingers in a saturated porous medium without change of total salt mass and possibly including the influence of heterogeneities.

The experimental set-up consisted of a container with impervious boundaries filled with glass beads as a porous medium. In the upper central part of the homogeneous bead packing, a heterogeneity was introduced by embedding a more permeable blockshaped zone. An unstable saltwater/freshwater layering serves as initial condition (see Fig. 2). It was produced by removing a thin plastic sheet separating the salt and fresh water zones at time t=0. The inner size of the cube-shaped container was 240 mm along each edge. The upper third was filled with a salt solution of concentration c = 3 g/l. The highly permeable zone was 40 mm by 40 mm in the horizontal directions and 160 mm in the vertical direction.

The value of the nondimensional Rayleigh number (*Ra*) (for a horizontally infinite, homogeneous porous medium) exceeded $4\pi^2$ (Eq. 1). On the basis of this criterion in our case even a salt distribution increasing linearly from the bottom to the salt/freshwater interface would show instability. The Rayleigh number including the damping effects (λ) of sidewalls according to *Wooding* (1959) is also larger than its critical value due to the narrow transition zone (see also *Bachmat and Elrick*, 1970). Hence, some kind of convective mixing must develop.

$$Ra = \frac{\Delta\rho \cdot k \cdot g \cdot H}{n \cdot \mu \cdot D} \quad \text{and} \quad \lambda = \frac{d\rho}{dz} \cdot \frac{k \cdot g \cdot a^2}{\mu_m \cdot D} \qquad (1)$$

where n is porosity, k the permeability, D the effective diffusion coefficient, μ and μ_m the viscosity and the mean viscosity respectively, ρ the density and g the gravitational acceleration. The geometry of the container is characterised by its height H and a is a typical length taken as half the width. The Rayleigh number is, however, in some cases not sufficient to describe interfacial stability (*Schincariol et al.*, 1994).

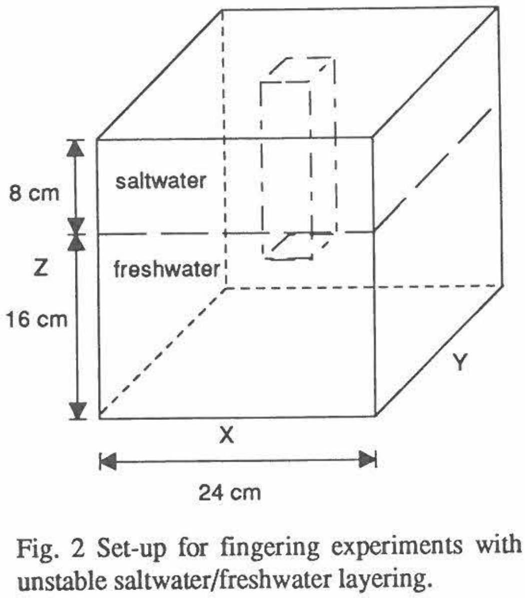

Fig. 2 Set-up for fingering experiments with unstable saltwater/freshwater layering.

We used a nuclear magnetic resonance apparatus to get time-dependent concentration data in three dimensions. Copper sulphate ($CuSO_4$) was added to the saltwater as a paramagnetic tracer in low concentration to get a linear signal-to-concentration relation. The magnetic resonance imaging (MRI) was performed in slices of 5 mm thickness with an image plane resolution of 2.34 mm using a spin-echo imaging sequence.

After removing the separating plastic sheet, the denser saltwater flows downward forming fingers, while the fresh water is forced to go up in a similar way. Additionally, there is mixing by diffusion and dispersion. The built-in block of higher permeability acts as a preferential location for finger flow (see Fig. 3). Starting out with a very small size the fingers do not only grow in length but also in width. The latter phenomenon is caused by dispersion and the coalescence of smaller fingers. Also tipsplitting is visible. The primary and quickest flow of saltwater takes place in the highly permeable zone accompanied by upward freshwater fingers in the same zone. In the low permeability region fingering is observed over the whole horizontal plane. Their development, however, is significantly slower. Hence the convective, vertical mixing by the miscible fingering is dominated by the heterogeneity, although this zone is small in size compared to the whole cross-section. Although the extension of the highly permeable zone in the vertical direction was limited, the vertical finger movement was not stopped when the finger reached the bottom of this zone. Finger width increased still further.

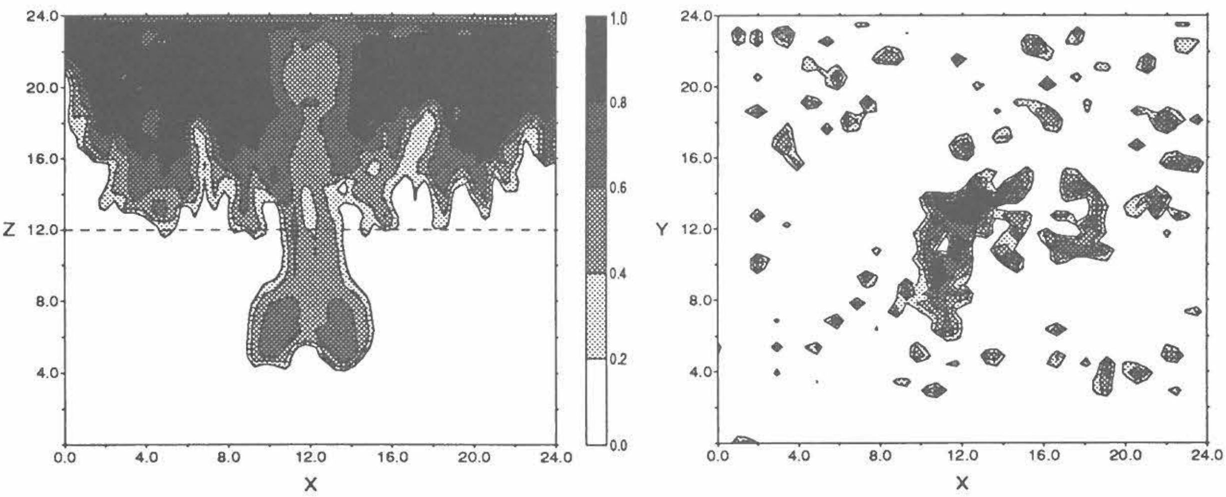

Fig. 3 Fingering of saltwater in unstable layering with central heterogeneity (a) Vertical centre plane, permeability ratio of 5.1, after 176 minutes; (b) Horizontal plane, permeability ratio of 3.2, 4 cm below initial interface as indicated in 3a (dotted line), after 166 minutes.

Benchmarking on the basis of this unstable type of flow phenomenon has to be different from the usual comparison of local concentrations, heads, or velocities applied in stable problems. A comparison between model and measured data has to focus on the generic properties such as the geometry of the basic evolving flow pattern. What can be compared are quantities such as finger growth speed, finger size (as done by *Manickam and Homsy*, 1995) and spatial frequencies or onset of fingering and fingering modes as a function of the Rayleigh number. To reproduce these features is a challenge for numerical flow codes and modelling, yet it presents the most sensitive test whether the physical nature of the problem is captured by the model.

An example of the results of numerical simulation of the experiment discussed above is shown in Fig 4. We used the code SALTFLOW (*Frind and Molson*, 1994). This code was able to reproduce the development of fingers in the highly permeable heterogeneity starting with a sharp initial interface between saltwater and freshwater. But it did not show any fingering in the outer, low permeable part of the porous medium.

This is due to several reasons. Firstly, the actual initial perturbations of the interface (caused by pulling out the plastic sheet) and the unavoidable small variations of permeability and porosity in the physical model, which constitute the origin of fingers, were not taken into account. Further, the density gradient at the front may be reduced in the model due to limited resolution.

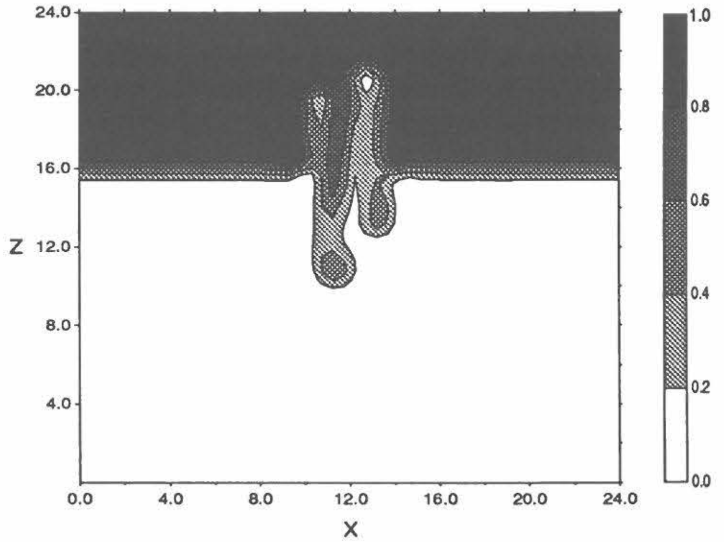

Fig. 4 Calculated concentration in the central vertical cross-section; permeability ratio 5.1, after 173 minutes.

A comparison of the finger length development of the central finger (Fig. 5) indicates that the numerical calculation is able to reproduce the correct growth rate of the finger, but a much longer time is necessary for fingering to start. Both, experimental and numerical results show a linear growth rate of finger length, which coincides with results of similar experiments (*Pearl*, 1993).

Applying a small perturbation of the salt concentration to the initial interface could shorten the time lag of finger initialisation, provided it has an appropriate wavelength. In this case, too, there is no finger growth in the outer part of the model yet. The main problem in modelling finger development is to obtain the observed onset of fingering. This demands a very high degree of grid resolution in the interface region, use of an appropriate initial perturbation and numerical codes, which do not suppress or smear out small differences in concentration or head. On the other hand, the simulation of finger growth after initiation seems to be possible.

Apart from its use in the validation of codes, density flow and fingering on a small scale is of interest in itself, because it may influence flow and transport also on a larger scale by increasing - or in some cases even decreasing - vertical mixing, particularly under heterogeneous conditions. Hence, investigating fingering in laboratory experiments and numerical simulation should help to find an appropriate way to account for the subscale effects in large scale modelling using effective parameters.

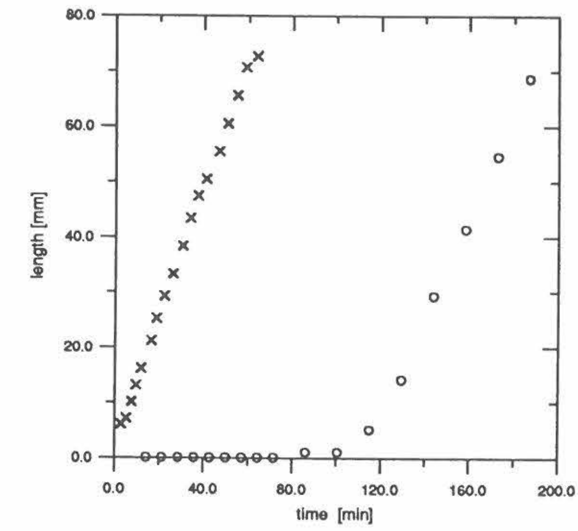

Fig. 5 Finger growth of central finger: Comparison between experimental data (denoted by crosses) and numerical simulation (denoted by circles).

Proposed benchmark

To have a benchmark test, which does not demand as much from the transport code and the physical modelling approach as the fingering example, we suggest another problem case (see Fig. 6). It starts from a stable sharp interface saltwater/freshwater layering with no inflow. The change in salt distribution and flow field under the influence of a constant influx/discharge of freshwater presents a situation useful for benchmarking. This problem is not only closely related to the situation of transient mixing of freshwater with saltwater in case of seawater intrusion, but also to salinization of an aquifer in the neighbourhood of a salt dome.

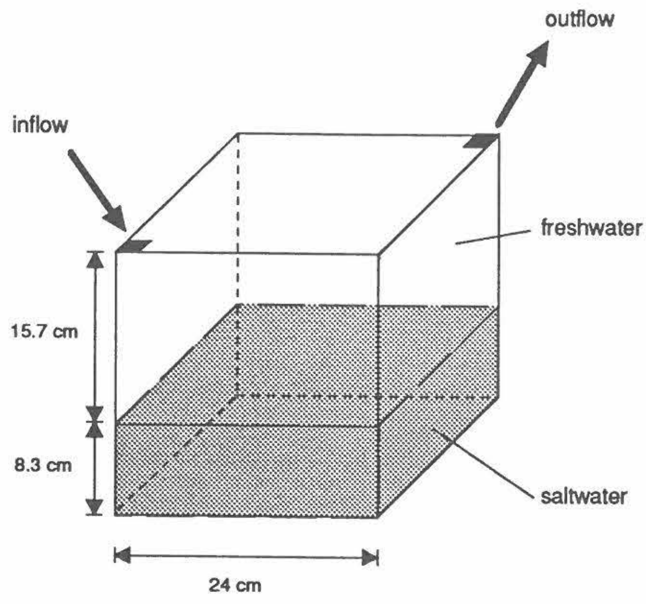

Fig. 6 Saltwater pool at the bottom of an impervious container with inflow and outflow at top corners.

As numerical calculations indicate there can be different flow patterns depending on the physical parameters: In the case of high freshwater discharge and low salt concentration the saltwater can be displaced easily by the freshwater flow, whereas in the opposite case a saltpool will remain at the bottom. Inside the saltwater zone one or more eddies develop driven by the flow field above the interface. Now, the saltwater is transported upward by dispersion and diffusion only, thus forming a transition zone (Fig.7a and b).

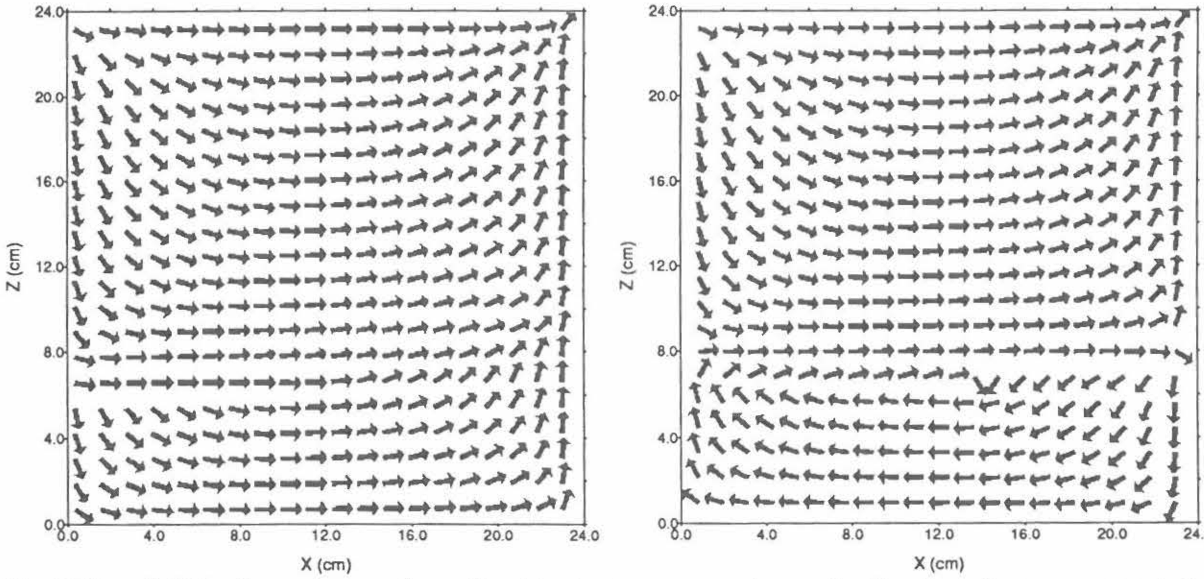

Fig. 7 Flow field in the centre xz-plane after 14 minutes, arrows show only direction of x,z components (a) initial salt concentration at the bottom is 100 g/l, total inflow/outflow is 0.1 l/min. (b) initially saturated brine (300 g/l) at the bottom, same inflow/outflow as in (a).

In contrast to the Henry problem, here the time evolution of an already existing saltwater layer after introduction of a freshwater inflow is studied. No nontrivial steady state solution exists. This choice takes into account that the insensitivity of the Henry problem is not only caused by the stability of the stratification but also by the fact that in this steady state situation numerical diffusion does not play a role. Additionally the possibility of different resulting flow and concentration patterns depending on inflow, dispersion, and initial salt concentration provide a tool to judge the capabilities of transport codes in this benchmark. The problem set-up is also well-suited for investigation with MRI as was the case in the fingering example shown above.

Conclusions

The Henry problem can only be used as a very weak benchmark for the general capabilities of transport codes for density driven flow. To validate such codes comparison with generic properties of fingering phenomena can be used, also in three dimensions. A time-dependent, three-dimensional, stably layered problem with external inflow and outflow could be a promising benchmark.

Acknowledgements

This work is financially supported by the GRS, Cologne. We want to thank Dr. G. Brix (German Cancer Research center DKFZ, Department of Radiological Diagnostic and Therapy, Heidelberg, Germany) and Andrea Greiner (Inst. of Environmental Physics, Heidelberg, Germany) for their contributions in performing the MRI measurements and Philippe Ackerer/Anis Younes (Inst. de Mécanique des Fluides, Strassbourg, France) and Gabi Beddies (Inst. for Computer Applications, Stuttgart, Germany) for their calculations of the Henry problem.

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