FEMLAB® Performance on 2D Porous Media Variable Density Benchmarks

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1 Introduction

Variable density problems are suitable test-cases for multi-physics codes, as the interaction between flow and transport processes is a characteristic of the observed phenomena. Fluid properties density and viscosity are influenced by temperature and/or salinity and deliver the feedback from transport to flow. Other parameter dependencies may contribute in addition. In porous media porosity and permeability may also depend on temperature or salinity. Variable density problems offer a wide variety of phenomena: onset of convective motions, either steady state, oscillatory or chaotic, penetration of saltwater wedges, fingering, interaction with additional external regimes, etc.

Test-cases are accepted in the modelling community as benchmarks, when they have been used for testing in several publications. This contribution focuses on density-driven flow benchmarks in porous media. Several test-cases have been proposed by various authors, which will not be treated in detail. Here FEMLAB® results are shown for the Henry model concerning stationary saltwater intrusion, and the Elder heat convection experiment in a Hele-Shaw cell. A brief introduction is given concerning the saltdome problem.

First follows an overview on systems of differential equations, which are appropriate for studies on variable density flow patterns, depending on the validity of simplification assumptions. Set-up and output of FEMLAB ® models for two of the three mentioned test-cases are presented. The study shows that FEMLAB® is a powerful tool that delivers performs well on the benchmarks. Important in comparison to other software packages is the fact that the models can be set-up most easily in the FEMLAB® graphical user interface.

2 Differential Equations

In variable density problems flow and transport are coupled; in usual flow and transport problems they are not. The general flow equation in 1D, 2D or 3D problems is given by:

$$\frac{\partial}{\partial t}(\varphi\rho) = \nabla \cdot (\rho \frac{\mathbf{k}}{\mu}(\nabla p - \rho \mathbf{g})) \tag{1}$$

with porosity φ, density ρ, viscosity μ, pressure p, the gravity vector $\mathbf{g}$ and the permeability tensor $\mathbf{k}$. In porous media the relevant Darcy-velocity $\mathbf{v}$ is given by the equation:

$$\mathbf{v} = \frac{\mathbf{k}}{\mu}(\nabla p - \rho \mathbf{g}) \tag{2}$$

Transport concerns component mass or heat. The mass transport equation in 1D, 2D or 3D problems is given by:

$$\frac{\partial}{\partial t}(\varphi\rho c) = \nabla \cdot \rho(\varphi \mathbf{D} \nabla c - (\mathbf{v}c)) + q_c \tag{3}$$

with concentration c and sink/source-term q_c and where $\mathbf{D}$ denotes the dispersion tensor:

$$\mathbf{D} = \left(D_{ij}\right) = \left((D + \alpha_T v)\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{v} \right) \tag{4}$$

with mass diffusivity D, longitudinal dispersivity α_L and transversal dispersivity α_T. The heat transport equation is:

$$\frac{\partial T}{\partial t} = \nabla \cdot (D_T \nabla T - (\kappa \mathbf{v} T)) + q_T \tag{5}$$

where T denotes temperature, D_T the thermal diffusion coefficient of the fluid/solid system and κ the ratio of heat capacities of the fluid in comparison to that of the fluid/solid system. q_T denotes heat sinks or sources.

The transport is always dependent on the solution of the flow equation, as the velocity v determines advective transport. The link from transport back to the flow equation, which can be neglected in usual applications, is given through the dependencies $\rho(c,T)$ and $\mu(c,T)$, the dependences of density and viscosity on salinity and temperature.

In most the system of generic equations, as formulated above, is not treated directly. Especially in older publications the system of equations. The most common simplification is the so called Oberbeck-Boussinesq assumption, which states that density differences are relevant at first place in the so called buoyancy term of the Darcy equation and can be neglected everywhere else (Holzbecher 1998a). This assumption concerns equations(1) and (3)

Further assumptions can be made to argue for further simplifications of the system of differential equations. In 2D the flow equation can be formulated in terms of the streamfunction Ψ (instead of pressure):

$$\frac{\partial}{\partial x}\left(\frac{\mu}{k_z}\frac{\partial \Psi}{\partial x}\right) + \frac{\partial}{\partial z}\left(\frac{\mu}{k_x}\frac{\partial \Psi}{\partial z}\right) = -g\frac{\partial \rho}{\partial x} \tag{6}$$

where x and z denote the horizontal and vertical space directions, k_x and k_z the corresponding permeabilities (Holzbecher 1998). Velocities and streamfunction are connected by the formulae:

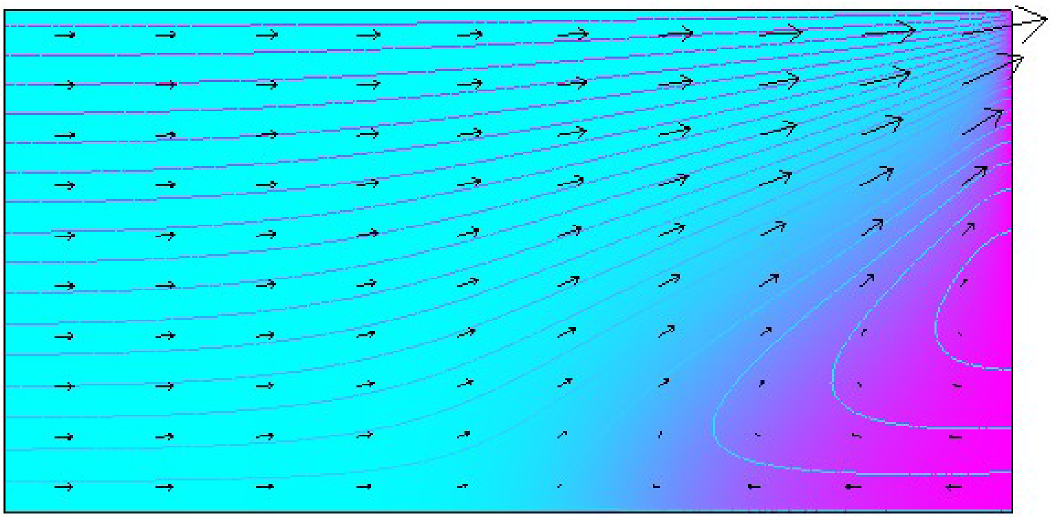
$$\frac{\partial \Psi}{\partial x} = v_z \qquad \frac{\partial \Psi}{\partial z} = -v_x \tag{7}$$

Another formulation, in terms of an equivalent hydraulic head, is also found in the literature; for details see Holzbecher (1998a). The multi-physics FEMLAB® has the advantage that all types of equations can be taken in the multi-physics

3 Saltwater Intrusion (Henry-Testcase)

The first benchmark for variable density flow is the Henry test-case (Henry 1964), which is based on an idealized and simplified situation, where saltwater enters an aquifer at the base. The constellation is relevant in ocean coastal regions or in the vicinity of inland saline water bodies, as salt-lakes.

The model region represents a 2D cross-section through a confined aquifer. There is an inflow of fresh water across the vertical boundary at one side, while on the opposite vertical boundary a constant high salinity concentration is required. The flow boundary condition at these edges is that there are no vertical velocity components. Top and bottom boundaries are closed.



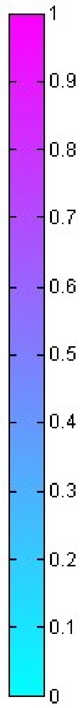


Figure 1. Results for the saltwater intrusion (Henry) testcase; fresh water (c=0), entering from the left, is squeezed between the upper boundary and a saltwater (c=1) wedge, entering from the right; surface plot represents salinity; depicted streamlines are calculated as contours of the streamfunction; arrows are calculated form the velocity field, using streamfunction derivatives (eq. (7))

The idealized situation, described by Henry, has attracted much attention as a test-case for steady state variable density flow and transport. Selected references are: Pinder & Cooper (1970), Lee & Cheng (1974), Ségol *et al*. (1975), Frind (1982), Voss & Souza (1987), Paniconi & Putti (1993), Ségol (1994), Croucher & O'Sullivan (1995), Kolditz *et al*. (1998), Holzbecher (1998a), Benson *et al.* (1998), Oldenburg & Pruess (1999), Simpson & Clement (2003, 2004).

Figure 1 illustrates the resulting flow pattern for the Henry test-case, calculated with FEMLAB®. Following a parallel flow field fresh water is entering from the left. While approaching the saltwater boundary on the right, the fresh water flow becomes squeezed between the upper boundary and a saltwater wedge, entering from the right near the aquifer base. Between fresh- and saltwater a mixing zone emerges.

The FEMLAB® model is based on a grid of 12682 elements, obtained by using the 'adaptive grid' option. For the simulation the streamfunction formulation, as given in eq. (6), was chosen – similar to the original formulation of Henry (1964). For the case of constant parameters the system of differential equations can be reduced to the combination of a Poisson equation and a convection-conduction equation. The result of FEMLAB® coincides with recently published output of other modelling approaches with refined grids and reduction of numerical dispersion (see references cited above).

4 Unsteady Convection (Elder Experiment)

Elder (1967) published results of several experiments, performed in Hele-Shaw cells. These are closed cavities, in which a viscous fluid fills the thin (several mm) space between two plates. In one of Elder's experiments the fluid between the two vertical plates was heated from below. In contrast to classical experiments of convection only the middle part of the lower boundary was heated.

The Elder experiment has been used as a benchmark by numerous modellers concerned with variable density flow in porous media (Horne & O'Sullivan 1974, Kolditz 1994, Kröhn 1994, Oldenburg & Pruess 1995, Kolditz *et al*. 1998, Holzbecher 1998a, Ackerer *et al*. 1999, Oltean & Buès 2001, Frolkovič & De Schepper 2001, Johannsen 2002, Simpson & Clement

(2003). The background is that highly viscous Hele-Shaw flow behaves similar to porous media flow, which follows Darcy's Law. The experiment was included as a test case in the international HYDROCOIN project (1988, 1990), a project concerned with modeling for safety assessment of nuclear waste facilities. Concerning the different variants of the Elder problem, found in the literature, it is important that a similar influence on the density can be induced either by salt concentration or by temperature. The difference is that in the saline case the fluid is salted at the top, instead of being heated at the bottom. One should be careful, to take the similarity too far, as thermal and saline dispersion are not identical (see section 2).

In FEMLAB® the experiment can be treated in different ways, concerning the simplifications mentioned in section 2: one may use the full set of equations, the simplified form according to the Oberbeck-Boussinesq assumption or the further simplified form using the streamfunction. Another alternative, using the 'Earth Science Module' of FEMLAB®, is demonstrated in a FEMLAB® tour CD (2005), in which the Oberbeck-Boussinesq assumption is utilized for the transport equation (3), not for the flow equation (1).

Figure°2 depicts the flow pattern obtained using FEMLAB 3 for the simplified approach based on the streamfunction formulation for the thermal case. The adaptive grid option was utilized, resulting in a highest grid refinement near the position, where heated and non-heated parts of the lower boundary meet.

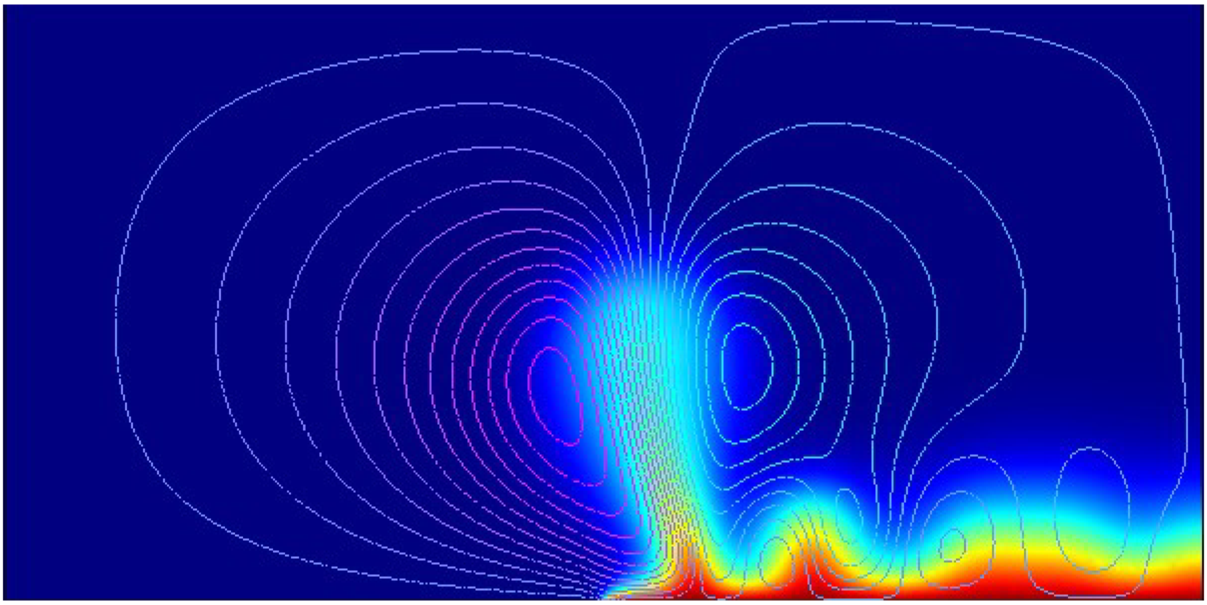


Figure 2. Results for the Elder experiment testcase after the onset of convection in the left half of the entire system; calculated for dimensionless time τ=0.01; surface plot shows temperatures (blue = low; red = high); contour lines for streamfunction represent temporary flow pattern (FEMLAB 3.1)

Tab. °1: Overview on results concerning the Elder testcase using FEMLAB; columns 4-8 list no. of visible eddies in the system at 5 time instants; § τ=0.075; two entries in a cell indicate that at least two minor eddies exist, which are not visible in a visualization with a small no of contours.

Case	**Nodes**	**Elements**	**τ=0.01**	**τ=0.02**	**Eddies τ=0.04**	**τ=0.07**	**τ=0.1**	**Comments**
Elder			4	8		2 / 4§	2	orig. paper
1	219	389	14	8	4	4	4	FEMLAB 2.3
2	826	1556	12	8	12	2	2	"
3	1083	2060	12	8	10	4	4	"
4	4225	8240	14	10	6 / 8	2	2	"

Comparison of FEMLAB® results for various degrees of grid refinement, as listed in Table 1, demonstrate that solutions are high sensitive to numerical parameters, noted as well by other modellers. The list shows that basic features, here the total number of eddies that are visible in the graphical output, depend on grid refinement. Figure 2 visualizes 6 eddies in the half-system, corresponding to 12 eddies in the entire system. The difference in the number of eddies even at final time (τ=0.1), received by FEMLAB® for different grid resolutions, reflects the disagreement in the scientific discussion about the valid final state of the Elder experiment.

5 The Saltdome Test-Case

Another benchmark that has been treated in literature is the so-called saltdome test-case, where ambient groundwater flow has contact with the top of a saltdome at the base. The problem was originally stated within the international HYDROCOIN workshop (HYDROCOIN 1988, 1990), and was discussed in the scientific literature by Herbert *et al*. (1988), Leijnse (1992), Oldenburg & Pruess (1995), Konikow *et al*. (1997), Kolditz *et al*. (1998), Holzbecher (1998a, 1998b), Younes *et al*. (1999). Using FEMLAB® a model of the saltdome problem can be set up with similar ease as demonstrated for the Henry- and the Elder problem. FEMLAB® results coincide with output from other high resolution models.

6 Conclusions

FEMLAB® is a perfect simulator for problems of variable density flow in porous media, as shown by results on benchmark problems. Most striking is the ease with which multi-physics models can be set up using the FEMLAB® graphical user interface.

FEMLAB® should be applied for further examinations of variable density benchmarks, for which there are still several open questions. FEMLAB® is an ideal tool for studying the differences stemming from using different formulations of differential equations. Moreover the influence of variable viscosity, which is neglected in most benchmark formulations, can be studied easily. It also may be crucial, how dispersivity is defined in the transport equation: does it make a difference, when the full dispersion tensor, as defined in eq. (4) is used instead of the simple diffusivity scalar?

Some other potential benchmarks for slightly more complex situations could not be mentioned here: free and forced convection, geothermal flow (Yusa test-case) and bubble motion. Moreover FEMLAB® is an ideal tool for treating more complex situations, like thermohaline convection, Dufour or Sorêt effects.

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