BENCHMARK CALCULATIONS OF VARIABLE-DENSITY FLOW IN POROUS MEDIA

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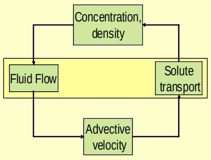
Variable-density flow problem

Governing equation and modelling

Variable-density porous media flow problem is coupled problem of water flow and solute transport: the water velocity as a result of the flow problem is a parameter in the solute transport problem (standard case) and the solution density as a parameter in the flow problem is dependent on concentration, result of the transport problem (specific for variable-density flow). (Figure)

Due to the flow-transport coupling, the problem is also non-linear.



It is one of the challenges of the groundwater modelling and numerical mathematics (Holzbecher 1998, Dierch and Kolditz 2002.).

The porous media water flow is governed by the generalised Darcy's Law and the mass balance equation (Bear and Verruijt 1990). We use the usual Oberbeck–Boussinesq approximation, neglecting the variable-density terms in the mass balance equation [Oltean and Bues 2001]. In contrast with the constant-density porous media flow, the problem is no more represented as potential field.

Standard porous media flow	Variable-density porous media flow
$\kappa(h)\dfrac{\partial h}{\partial t} - \nabla\cdot(K\nabla h) = q$	$\kappa(h)\dfrac{\partial h}{\partial t} - \nabla\cdot(K(\nabla h + \varrho_r\nabla z)) = q$
$\boldsymbol{u} = K\nabla h$	$\boldsymbol{u} = K(\nabla h + \varrho_r\nabla z)$

Auxiliary variables

$$\varrho_r = \frac{\varrho-\varrho_0}{\varrho_0} \qquad \nabla z = \frac{\boldsymbol{g}}{|\boldsymbol{g}|} \qquad h = \frac{p}{\varrho_0 g} + z$$

The considered mechanisms of porous media solute transport are
- advection in the mobile zone
- hydrodynamic dispersion in the mobile zone
- diffusion exchange between the mobile and the immobile zones (blind pores)

$$\frac{\partial c_m}{\partial t} + \nabla\cdot(c_m v) - \nabla\cdot(D\nabla c_m) = \frac{1}{n_m}\alpha(c_i - c_m) + c^* q_s^+ + c_m q_s^-,$$

$$\frac{\partial c_i}{\partial t} = -\frac{1}{n_i}\alpha(c_i - c_m),$$

u	Darcy velocity	c_m	mobile concentration
v	seepage velocity, $v=u/n_m$	c_i	immobile concentration
h	piezometric head	c^*	injected concentration
p	pressure	q_s^+	fluid source intensity
K	tensor of hydraulic conductivity	q_s^-	fluid sink intensity
ρ	solution density	D	tensor of hydrodynamic dispersion
ρ_0	reference density	α	rate of mobile-immobile exchange
ρ_r	relative density	n_m	mobile porosity,
z	vertical coordinate	n_i	immobile porosity
g	gravity acceleration	n	total porosity ($n = n_m + n_i$)

Abstract

We deal with the variable-density porous media flow problem, i.e. coupled flow and advective-diffusive solute transport. We present results of numerical simulations of a particular benchmark problem, comparing the density-coupled model with the uncoupled one, two different finite-element approximations, influence of discretisation size, and influence of physical parameters (intensity of coupling).

In a similar discretisation structure composed of trilateral prismatic elements and derived from unstructured triangulation in the horizontal projection, we use two different numerical schemes, one based on the mixed-hybrid finite elements and the second based on the combination of 2D linear finite elements and 1D finite differences. The variable-density coupling is implemented as a simple iteration loop.

The benchmark is constructed according to the real hydrogeological configuration in Stráž pod Ralskem in the northern Bohemia, a site of former uranium leaching. The numerical results confirm the strong influence of physical parameters and vertical discretisation. The differences between studied numerical schemes and discretiastions are smaller.

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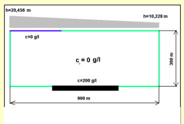
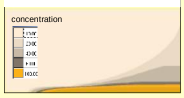
Variable-density benchmarks

During the past decades, several standard benchmark problems has been used. They are mostly constructed as a simplification of coastal water reservoirs with mixing of freshwater and salt water. Up to very specific exceptions, the problems do not have analytical solutions and are used to compare the numerical schemes between each other.

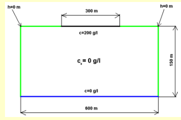
Saltdome problem: The problem with real-scale dimension used in the HYDROCOIN project (Holzbecher 1998). The configuration is clear from the figure: the flow field (given by pressure head *h* boundary condition) drives the solute to the right top corner while the gravity drives the denser solution (concentration *c*) downwards.



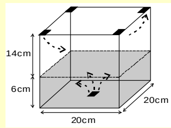
Henry problem: One of the oldest benchmark. Similar configuration to the saltdome problem. There exist an analytical solution but later found as incorrect (Dierch & Kolditz 2002). According to arguments that the problem should be sensitive enough to the presence of coupling, the problem is not suitable for numerical testing (Simpson & Clement 2003).



Elder problem: The problem is specific with its complicated (chaotic) behaviour. E.g. the number of upwelling and downwelling streams is dependent on the numerical scheme and discretisation step (Diersch & Kolditz 2002, Simpson & Clement 2003).



Saltpool problem: The newest of the cited benchmark, three-dimensional. It is specific with the laboratory-scale dimensions. The data from the laboratory measurement are available for the testing of numerical codes (Johannsen et al. 2002). The configuration resembles the "saltdome problem".



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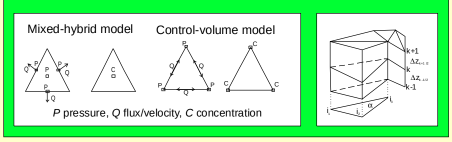
Numerical schemes and codes

Structure of the discretisation and positions of the discrete unknowns



Mixed-hybrid finite-element scheme

The principle of the method is outlined in the more precise name of the method, i.e. hybridised mixed FEM: the unknowns are pressures, fluxes (discrete form of velocity), and the Lagrange multipliers (with physical sense of pressure) corresponding to the constraint of conservative fluxes between elements. For detailed mathematical formulation of MHFEM on trilateral prismatic elements we refer to Maryška et al. (1995); for general description of mixed and hybrid methods see Brezzi and Fortin (1991).

Lowest-order approximation spaces:
- the pressure is approximated by piecewise constant function (in elements),
- the Lagrange multipliers ("pressure on sides") by piecewise constant functions (on structure of inter-element interfaces),
- the velocity by linear vector functions (Raviart-Thomas space, see Kaasschieter and Huijben 1990).

Algebraic problem:
Symetric semidefinite

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C} \\ \mathbf{B}^T & & \\ \mathbf{C}^T & & \mathbf{S} \end{bmatrix} \begin{bmatrix} \mathrm{U} \\ \mathrm{P} \\ \Lambda \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \\ \mathbf{q}_3 \end{bmatrix}$$

The solver used in our model is based on Schur complement reduction and conjugate gradient method (see Maryška et al. 2000).

The **variable-density term** appears as additional RHS term (no special technique needed:

$$\sum_{e\in E_h}\{-<p_{1,h},\mathbf{n}^e\cdot\mathbf{v}_h>_{\partial e\cap\partial\Omega_1} - <\rho gz,\mathbf{v}^e\cdot\mathbf{n}^e>_{\partial e} + (\rho gz,\nabla\cdot\mathbf{v}^e)_{0,e}\}$$

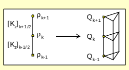
The corresponding coupled transport problem is solved by the finite volume upwind scheme, the algorithm together with the dual-porosity transport is described in Hokr et al. (2003).

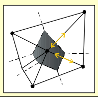
Control-volume finite-element scheme

Standard FEM with linear base functions understood as finite volume method on dual mesh, i.e. With control volumes associated with mesh nodes.

Provides mass conservation with respect to the dual mesh. In the particular case of the mesh of trilateral prisms (or system of layers with joint triangulation) we use the following technique (see Hokr and Wasserbauer 2004):
- Discretisation separately in the horizontal direction and in the vertical direction
- In the horizontal layers we apply the FEM with linear base functions on triangles
- finite differences in the vertical direction
- This method is algorithmically processed using the local matrices 6x6.

The variable-density (gravity) term is discretised consistently with the mass-conservation property (Hokr and Wasserbauer 2004a).

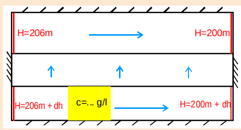




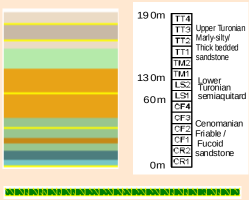
New benchmark formulation and numerical results

Benchmark configuration

Boundary conditions



Vertical and horizontal discretisation



Benchmark features

- Quantitative evaluation (clear interpretation of competitive driving forces of hydraulics and gravity), variable input parameters
- Real-world counterpart (see attachment), possible availability of field measurement data, artificial contamination instead of salt
- Simple boundary conditions

Possible drawbacks:
- Influence of initial condition
- Uncertainty with the time interval (no steady state)
- Choice of single representative measure

Problem evaluation

- C(x,z,t) distribution of concentration at final time t=200years
- Sum of mass in each layer: simple measure of vertical distribution, comparison of down/up driving forces

Problem parameters

Discretisation:
- original (figure): Δz=7.5 - 30 (variable), Δx=20, 1400 elements
- Two levels of refinement: 5600 elements, 22400 elements

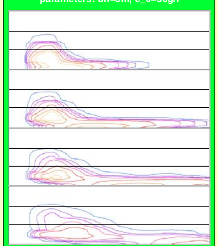
Initial condition:
Reference values of the non-zero concentration domain: 10g/l, 30g/l, 50g/l (inhomogeneous layer by layer).

Flow boundary condition:
Strength of the vertical hydraulic gradient: dh= 1m, 3m, 10m.

Model structure:
- Variable density (coupled)
- Constant density

Numerical method:
- Mixed-hybrid FEM (elements)
- Control-volume FEM/FVM (nodes)

Time history: 20, 50, 100, 200 years
parameters: dh=3m, c_0=30g/l



Isolines: 0.1; 0.5; 1; 2; 5; 10; 20 g/l

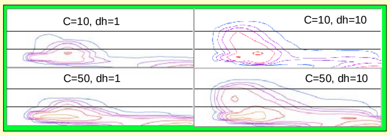
Physical parameters sensitivity

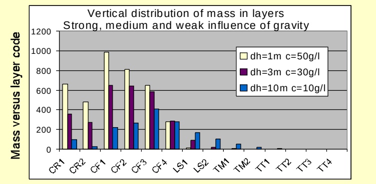
Mass transfer to the top (Turonian) aquifer

More ← influence of gravity → less; influence of gravity: less ↕ More

	bottom/top (Cenomanian-Turonian) head difference (m)					
Initial concentration	1		3		10	
g/l	ton	% initial	ton	% initial	ton	% initial
10	0,053	2,66E-03	2,491	0,12495	66,605	3,340941
30	0,025	4,87E-04	3,317	0,064664	110,101	2,146386
50	0,014	1,69E-04	3,403	0,041171	135,563	1,640087

Overall spatial distribution





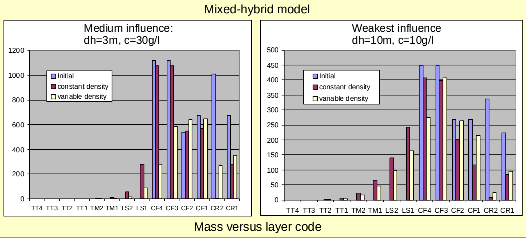
Discretisation sensitivity / Model sensitivity

Control-volume model

Vertical distribution of mass at time t=200yrs for medium gravity influence c=30g/l, dh=30m

	variable density			constant density		
	original	refinement 1	refinement 2	original	refinement 1	refinement 2
top layers	2,09424	0,544248	0,103917	11,3472	5,779908	1,651854
medium layers	64,43751	29,00689	18,38648	302,4194	315,125	321,7837
bottom layers	215,0734	235,7934	129,6829	400,604	503,5995	555,1438

Mixed-hybrid model



Mass versus layer code

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