# NUMERICAL ASPECTS OF DENSITY DRIVEN FLOW IN POROUS MEDIA

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## ABSTRACT

The analysis as well as the numerical simulation of density driven flow in porous media is still a challenging task. Whereas thorough theoretical investigations are limited to special situations, the numerical treatment, especially of real-world problems, requires special numerical techniques. In this contribution we focus on two aspects, which are relevant in this context. The first deals with the analysis and design of robust multigrid solvers. In the second part, we investigate a realistic saltwater intrusion problem. Its solution gives rise to a special type of numerical problems. Numerical results are presented confirming the theoretical findings.

## 1. INTRODUCTION

Density-driven flow in porous media is relevant in a number of frequently occurring problems such as sea-water intrusion in coastal aquifers, upconing of saline waters from deep aquifers, flow around salt domes used as repositories, propagation of dense plumes emanating from landfills and geothermal heat production. Even in cases of relatively low density-contrasts density effects cannot be neglected. In practice, this requires reliable and efficient methods for solving the coupled problems.

In this paper we focus on the design of robust multigrid methods and their application to a realistic sea-water intrusion problem. It is structured as follows. In section 2 we discuss briefly the governing equations. Subsequently, in section 3, we discuss numerical issues of the mathematical model and the design of fast solution methods required in this context. The emphasis is on multigrid methods. In section 4 the methods are used in application to a realistic sea-water intrusion problem. Numerical issues as well as results are discussed. Finally, in section 5 concluding remarks are given.

## 2. THE MATHEMATICAL MODEL

The governing equations for the coupled density-driven flow in porous media are derived from mass-conservation principles. Assuming incompressibility of the fluid, the following system results (Bear and Bachmat, 1991; Holzbecher, 1998; Leijnse, 1992).

$$\frac{\partial(n\rho(\omega))}{\partial t} + \nabla \cdot (\rho(\omega)\mathbf{q}) = Q_p(\omega), \tag{1}$$

$$\frac{\partial(n\rho(\omega)\omega)}{\partial t} + \nabla \cdot (\rho(\omega)(\omega\mathbf{q} - \mathbb{D}\nabla\omega)) = Q_\omega(\omega). \tag{2}$$

Flow equation (1) describes conservation of fluid mass, whereas transport equation (2) describes conservation of salt mass. With $n$ we denote the porosity, with $Q_p$ and $Q_\omega$ sources and sinks for the flow and transport equation resp. Density is denoted by $\rho = \rho(\omega)$, the diffusion-dispersion tensor by $\mathbb{D} = \mathbb{D}(\mathbf{q})$ and the mass-averaged velocity $\mathbf{q}$ is given by Darcy's law

$$\mathbf{q} = -K/\mu(\omega)(\nabla p - \rho(\omega)\mathbf{g}), \tag{3}$$

where $\mu = \mu(\omega)$ is the dynamic viscosity and $\mathbf{g}$ is the vector of gravity. Inserting Eq. (3) into Eqs. (1) and (2) leads to a nonlinear system of two partial differential equations (PDE's) for the unknown salt-mass fraction $\omega$ and the pressure $p$. To close the system, equations of state for $\rho$ and $\mu$, and an expression for the diffusion-dispersion tensor have to be provided. For $\rho$ and $\mu$, different dependencies are used in the literature, (Herbert et al., 1988; Holzbecher, 1998). We choose

$$\rho = \rho_0 e^{\gamma\omega}, \quad \gamma = 0.6923, \tag{4}$$

$$\mu(\omega) = \mu_0(1 + 1.85\omega - 4.1\omega^2 + 44.5\omega^3). \tag{5}$$

The density of freshwater is denoted by $\rho_0$. For the diffusion-dispersion tensor, we use Scheidegger's dispersion model (Scheidegger, 1961)

$$\mathbb{D}(\mathbf{q}) = nD_m\mathbb{I} + \alpha_t|\mathbf{q}|\mathbb{I} + (\alpha_l - \alpha_t)\mathbf{q}\mathbf{q}/|\mathbf{q}|,$$

where $\mathbb{I}$ denotes the unit tensor. We assume the validity of Fick's law and Darcy's law for our modeling approach. Boundary condition are either of Dirichlet- or of Neumann-type. For details, see (Hassanizadeh and Leijnse, 1988). Due to the assumed incompressibility initial conditions have to be specified only for the salt mass fraction.

## 3. DISCRETIZATION AND SOLUTION SCHEMES

The discretization and solution of the model equations are carried out using the program package d³f (Fein(ed), 1998; Johannsen, 2004).

For the spatial discretization of (1)-(3), we apply a vertex centered finite volume scheme with (multi-) linear ansatz functions on unstructured, hybrid, conforming grids consisting of tetrahedra, pyramids, prisms and hexahedra. We employ a consistent velocity approximation (Frolkovic, 1998). No stabilization is used for the convective terms. The discretization is second order consistent in the primary variables $\omega$ and $p$. For the discretization in time a diagonally implicit Runge-Kutta method of second order is used (Alexander, 1977).

The discretization leads to a sequence of nonlinear algebraic equations and by Newton's method to a sequence of large, sparse, linear equations. The latter are solved by a combination of a Krylov-subspace method using multigrid preconditioning (van der Vorst, 1992). Whereas the Krylov-subspace method is standard, the design of the multigrid method needs special attention.

3.1. **Characteristics of the Model Problem.** The solution of the discrete equations arising from the model equations in the context of realistic problems arising from environmental sciences is a challenging problem due to a number of reasons.

(1) Realistic models require a large number of unknowns due to the required high resolution and high accuracy.

(2) The problems are characterized by large jumps of the permeability $K$ of several orders of magnitude.

(3) Flow and transport phenomena are in general convection dominated with grid Peclet numbers of up to 50.

(4) The model geometries usually require unstructured, anisotropic grids with anisotropies of $1 : 10$ to $1 : 1000$.

(5) The discrete equations arising from systems of PDE's.

(6) Gravity effects.

Scientific Computing provides solution strategies for the problems (1)-(5) in case of simplified model situations. Solutions for problem (3) rely on stabilized discretization techniques (upwinding, limiter) or on stabilized iterative schemes (of ILU- and SOR-type). The former introduce further difficulties in the context considered here, the latter are recent developments and not well-established yet. Problem (6) is specific to the field of density dependent flow and transport and has not been recognized yet. Furthermore, the combination of these difficulties require an appropriate combination of solution strategies, which are in some cases mutually exclusive.

### 3.2. **Standard Solution Strategies.**
For the problems (1)-(5) solution strategies are available. We discuss them subsequently.

(1) The solution of large, sparse systems of equations, as they result from the discretization of PDE's, can be solved with optimal complexity using multigrid methods and high performance computers, see e.g. (Hackbusch, 1985). These methods are highly sensitive to the model characteristics. A stabilization with Krylov-subspace methods is mandatory for complex, nonlinear model problems.

(2) Jumping coefficients have to be resolved on the coarsest grid of the multigrid hierarchy. This leads to coarse grid problems of medium size, requiring special solvers, like optimized exact solvers, domain decomposition methods or algebraic multilevel methods. For an overview, see e.g. (Demmel et al., 1997; Ruge and Stüben, 1987; Smith et al., 1996).

(3) Convection dominated problems discretized by non-monotone schemes can be handled by either locally damped SOR-type or ILU-type iterations employing a special ordering, see (Johannsen, 2004).

(4) Scalar, anisotropic diffusion problems can be solved efficiently with a variant of the multigrid method using so-called robust ILU-smoothing, see (Wittum, 1989) and subsequent literature.

(5) Systems of equations can be handled by so-called point-block variants of iterative schemes.

The combination of these methods to a robust multigrid method able to handle the combination of these problems is possible, but requires special adjustments, see (Johannsen, 2004).

### 3.3. **Gravity Effects.**
Due to the nonlinearity of the transport equation its linearization exhibits an additional, virtual convection. This effect has not been recognized yet and is therefore discussed here in more detail.

We consider the linearization of the continuous operator $J$ defined by (1), (2). In the simplified setting of Boussinesq's approximation and a linear density we get after

appropriate scaling, while neglecting the linearization of the dispersion,

$$J \begin{bmatrix} \omega \\ p \end{bmatrix} = \begin{bmatrix} -\mathbb{D}(\mathbf{q}_0)\Delta\omega + (\mathbf{q}_0 + \omega_0\mathbf{q}_g) \cdot \nabla\omega & -\omega_0\Delta p \\ \mathbf{q}_g \cdot \nabla\omega & -\Delta p \end{bmatrix}, \tag{6}$$

where $\omega_0$ and $\mathbf{q}_0$ denote the salt mass fraction and Darcy velocity at the point of linearization, resp. The additional virtual velocity arises from gravity effects

$$\mathbf{q}_g = \frac{K\rho'\mathbf{g}}{\mu}, \tag{7}$$

whenever $\omega_0 > 0$. This virtual velocity may cause major difficulties for iterative solution schemes, including multigrid and Krylov-subspace methods. We consider a situation characterized by

$$D_m = 10^{-9}m^2s^{-1}, \quad K = 10^{-12}m^2, \quad \mu = 10^{-3}kgm^{-1}s^{-1}, \quad \alpha_l = 10m,$$

$$\alpha_t = 1m, \quad \rho' = 200kgm^{-3}, \quad \omega_0 = 3\%, \quad n = 0.35,$$

describing a realistic aquifer saturated with sea-water. The virtual velocity amounts to

$$\mathbf{q}_g \approx 2 \cdot 10^{-6}ms^{-1} \approx 62ma^{-1}. \tag{8}$$

We investigate a grid spacing of $H = 100m$ in the horizontal and of $h = 10m$ in the vertical direction. We consider two situations.

**Non-stagnant flow.** For the case of non-stagnant flow we assume a horizontal Darcy velocity of $|\mathbf{q}| = 50ma^{-1}$. The grid Peclet number $\mathcal{P}$ associated with Darcy velocity amounts to $\mathcal{P} = H/\alpha_l = 10$ (horizontal dispersion $\mathbb{D}_{xx}(\mathbf{q}_0) \approx \alpha_l\mathbf{q}_0$) and the grid Peclet number $\mathcal{P}_g$ associated with the virtual velocity amounts to

$$\mathcal{P}_g \approx \frac{|\mathbf{q}_g|h\omega_0}{\mathbb{D}_{zz}(\mathbf{q}_0)} \approx \frac{|\mathbf{q}_g|h\omega_0}{\alpha_t|\mathbf{q}|} \approx 0.4. \tag{9}$$

No essential difficulties arise in this case.

**Stagnant flow.** Here we assume stagnating flow ($\mathbf{q} = 0ms^{-1}$). In this case the dispersion vanishes and a grid Peclet number $\mathcal{P}_g$ associated with the virtual velocity of

$$\mathcal{P}_g = \frac{|\mathbf{q}_g|h\omega_0}{nD_m} \approx 1680 \tag{10}$$

results. Note that this Peclet number scales linearly with the permeability. A significantly large number therefore can be observed only for aquifers with a relatively large permeability. This case is typical for sea-water intrusion problems of islands and occurs frequently. Discrete problems with grid Peclet numbers of up to 50 can be handled efficiently by appropriate iterative solution schemes, like locally stabilized SOR-type or ILU-type schemes. The dominant convection discussed here needs a stabilization by small time-step sizes.
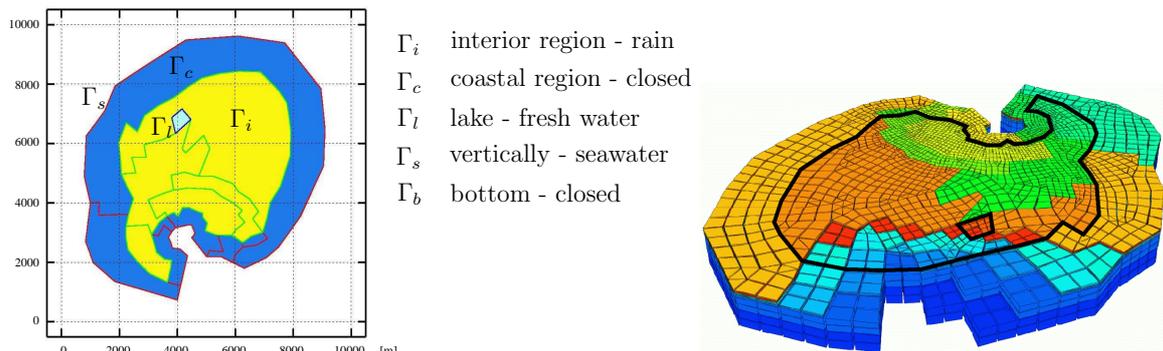
FIGURE 1. Left: Island Weizhou, schematic view from top. Boundary conditions are indicated by labels. Right: Coarsest grid used in the numerical simulations. Different hydrogeological layers are indicated by colors.

TABLE 1. Parameters.

| Parameter | Range | Unit |
|-----------|-------|------|
| K | $6 \cdot 10^{-15} \ldots 4 \cdot 10^{-12}$ | $m^2$ |
| n | $0.032 \ldots 0.22$ | - |
| $\alpha_L$ | $12 \ldots 521$ | m |
| $\alpha_T$ | $2.45 \ldots 31$ | m |

TABLE 2. The hierarchy of grids.

| Level i | # of elements | # of grid points |
|---------|---------------|------------------|
| 0 | 5248 | 5625 |
| 1 | 41.984 | 41.259 |
| 2 | 335.872 | 315.645 |

## 4. WEIZHOU-ISLAND: A SEA-WATER INTRUSION PROBLEM

In this section we investigate a sea-water intrusion and upconing problem. The Chinese island Weizhou is located in the Gulf of Tonkin, east of Vietnam. It has a diameter of about $10km$, its model problem a total depth of $800m$. It is made up of 8 layers with a thickness varying from $10m$ to $360m$. They contain 18 different hydrogeological units. The variations of some hydrogeological parameters are given in Table 1. A schematic view from top indicating the boundary conditions is given in Figure 1, left. The coarse grid used in the multigrid hierarchy contains 5248 elements (prisms, hexahedra) with aspect ratios varying from 1.5 to 600 and an average value of 30. It is displayed in Figure 1, right. We investigate numerical solutions obtained on a different grid-refinement levels, see Table 2. Sea-water with a maximum salt mass fraction of 2.5% is assumed. We investigate the sea-water intrusion into the island and subsequently an upconing process. Correspondingly we consider two phases.

4.1. **Phase 1.** At the beginning, we assume fresh water in the interior of the island ($\omega = 0$). Within the period of $\Delta T_1 = 10.000a$ simulated time sea-water intrusion leads to a stationary solution. For this period an average precipitation of $v = 0.393m/a$ is assumed. For grid level 1 a time-step size of $320a$, on grid level 2 a time-step size of $160a$, has been used leading an average Courant number of about 12 and maximum values locally of up to 380. Mean Peclet numbers of 3.3 on grid 1 and 1.7 on grid 2 occur with maximum value locally of up to 54 resp. 34. The virtual velocity (7) lead to Peclet numbers $\mathcal{P}_g$ of 900 on grid level 1 and 450 on grid level 2, cf. (10). Whereas discrete problems with Peclet numbers of up to $30 - 50$ can be solved a modified SOR iteration,
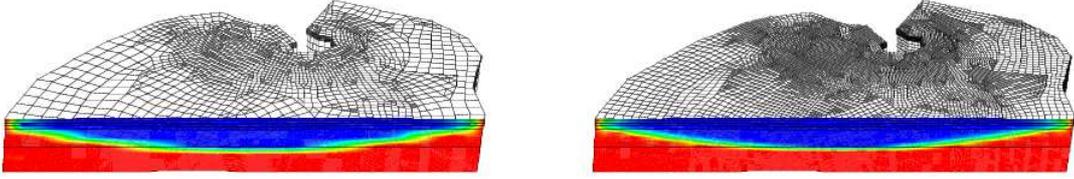
FIGURE 2. Salt mass fraction (stationary) on a vertical cross section at the end of phase 1. Left: Grid level 1, containing 41.984 elements. Right: Grid level 2, containing 335.872 elements.
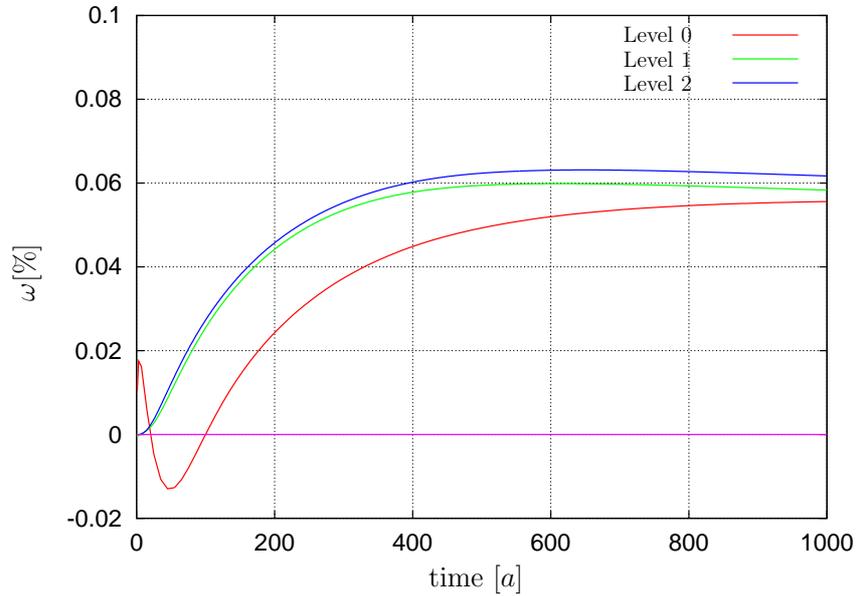


FIGURE 3. The breakthough curve of the well during phase 2. The different curves correspond to simulations on different grid levels, as indicated.

the virtual velocity with Peclet number of $\geq 450$ cause the time-step size restrictions observed in the simulation. The distribution of the salt mass fraction at the end of the phase on grid level 1 and 2 is shown in Fig. 2. The solution obtained on level 2 is accurate enough to allow for realistic predictions.

4.2. **Phase 2.** Subsequent to phase 1, we carried out simulations with one discharge well over a time period of $\Delta_1 = 1.000a$. It is positioned at the center of the island at a depth of $-100m$. The discharge rate of $q_1 = 9.5 \cdot 10^{-2} m^3 s^{-1}$ corresponds to 30% of the seeped rainfall. An upconing of sea-water could be observed. The breakthrough curves obtained on different grid levels are displayed in Fig. 3. Whereas the solution on grid level 0 is not accurate enough (large differences to the results on the finer grid levels, negative concentrations), the simulations on level 1 and 2 coincide fairly well, indicating that a further grid-refinement is not necessary. The salt mass fraction of the discharged water has an asymptotic value of 0.06%, i.e. is of drinking water quality. Fig. 4 shows the
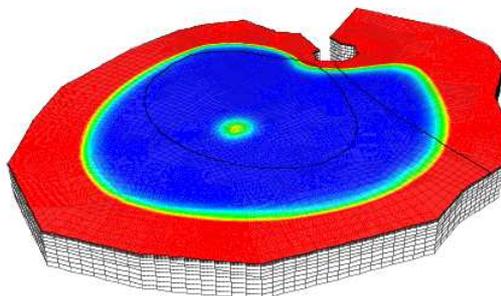
FIGURE 4. Salt mass fraction on the horizontal cross section at the end of phase 2, grid level 2.

distribution of the salt mass fraction on the horizontal cross section through the well at the end of the phase. The fresh water lense as well as the upconing in the neighborhood of the well can clearly be observed.

## 5. CONCLUSIONS

In this paper we have considered the numerical simulation of sea-water intrusion and upconing. Dealing with realistic model problems, a number of numerical issues have to be considered. It has been shown, that the major part of the numerical difficulties can be handled by (advanced) techniques from Scientific Computing. The only exception is a virtual convection arising from the linearization of discrete operators. Due to its destabilizing character is causes a significant time-step restriction for numerical simulations. We applied the methodologies to a realistic model problem and showed that sensible simulations are feasible.

## REFERENCES

Alexander, R. (1977). Diagonally implicit runge-kutta methods for stiff ode's. *SIAM J Numer Anal*, 14:1006–1021.

Bear, J. and Bachmat, Y. (1991). *Introduction to Modeling of Transport Phenomena in Porous Media*. Kluwer Academic Publishers.

Demmel, J., Gilbert, J., and Li, X. (1997). SuperLU users' guide. Technical Report CSD-97-944.

Fein(ed), E. (1998). d3f - Ein Programmpaket zur Modellierung von Dichteströmungen. *GRS, Braunschweig*, GRS - 139, ISBN 3 - 923875 - 97 - 5.

Frolkovic, P. (1998). Consistent velocity approximation for density driven flow and transport. *Advanced Computational Methods in Engineering, eds. R. van Keer et. al.*, pages 603–611.

Hackbusch, W. (1985). *Multi-Grid Methods and Applications*. Springer-Verlag, Berlin, Heidelberg.

Hassanizadeh, S. and Leijnse, A. (1988). On the modelling of brine transport in porous media. *Water Resources Research*, 24:321–330.

Herbert, A., Jackson, C., and Lever, D. (1988). Coupled groundwater flow and solute transport with fluid density strongly dependent upon concentration. *Water Resources Research*, 24:1781–1795.

Holzbecher, E. O. (1998). *Modeling Density-Driven Flow in Porous Media*. Springer-Verlag, Berlin, Heidelberg.

Johannsen, K. (2004). *Numerische Aspekte dichtegetriebener Stroemung in poroesen Medien*. Habilitationsschrift, Heidelberg University.

Leijnse, A. (1992). *Three-dimensional modeling of coupled flow and transport in porous media*. PhD thesis, University of Notre Dame, Indiana.

Ruge, J. and Stüben, K. (1987). Algebraic multigrid. *In: Multigrid Methods, S. F. McCormick (ed), Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania*, pages 73 – 130.

Scheidegger, A. (1961). General theory of dispersion in porous media. *Journal of Geophysical Research*, 66:3273.

Smith, B., Bjoerstad, P., and Gropp, W. (1996). *Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations*. Cambridge University Press.

van der Vorst, H. (1992). Bi-CGSTAB: A fast and smoothly converging variant of bicg for the solution of nonsymmetric linear systems. *SIAM J. Sci. Stat. Comp.*, 13:631 – 644.

Wittum, G. (1989). On the robustness of ILU smoothing. *SIAM J. Sci. Stat. Comput.*, 10:699 – 717.