Simulation and Parameter Identification of Oswald's Saltpool Experiments with the SAMG Multigrid-Solver in the Transport Code MODCALIF

F. Häfner

TU Bergakademie Freiberg, Akademiestrasse 6, D-09596 Freiberg, Germany,
email:frieder.haefner@tbt.tu-freiberg.de

K. Stüben

Fraunhofer-Institute for Algorithms and Scientific Computing (SCAI)
Schloss Birlinghoven, D-53754 Sankt Augustin, Germany, email:stueben@scai.fhg.de

Abstract The Saltpool experiments by Oswald & Kinzelbach (2003), carried out in 1998 at the ETH Zurich, are an excellent Benchmark test for numerical simulation programmes of the variable- density flow. Johannsen et al (2002) presented a detailed study that corresponded to the measurements after a parameter identification. The initial condition for phase 3 had to be estimated analytically due to the non-realistic thick transition zone after phase 2. The computing time for one simulation job amounted to about 20 h (16 Processor PC Pentium Cluster) for a grid of 274,625 points.

We continued the investigations by Haefner & Boy (2003) on a grid of 125,00 points where always the whole experiment (phases 1-3) is simulated. The thickness of the transition zone after phase 2 was very near to the observed value.

By incorporating the algebraic multigrid package SAMG as a linear equation solver, the overall performance could substantially be improved. A model calibration was carried out for the experiments case 1 and case 2 with the combination MODCALIF-SAMG which basically corroborated the results by Johannsen et al.

Without calibration a distance-depending dispersivity after Rösler & Schwan (1987) had also led to a good agreement with the observed concentrations.

Key words variable density flow; simulation; model calibration; saltpool experiment; samg-solver.

INTRODUCTION

The Saltpool experiments by Oswald (1999), described in detail by Oswald & Kinzelbach (2003), represent very good Benchmarks for the density-dependent mass transport with an essential influence of dispersion. A number of groups of scientists developing software for ground water flow and transport processes used these experiments as test examples. Here, it should be referred to the works by Diersch (2002) with the programme FEFLOW, Johannsen et al (2002) with d^3f, and Häfner & Boy (2003) with MODCALIF. There always arose three difficult problems in the numerical simulation of the experiments: (1) the initial parameter set by Oswald (1999) does not supply the measuring results (above all they do not supply the temporal course of the outlet concentration), (2) the concentration distribution at the end of phase 2 (rest period) shows smeary concentrations compared with the measuring results, and (3) the computing times for the simulation of one single experiment are very long, and consequently a model calibration with a frequent repetition of the simulation is nearly not feasible.

This work tries to solve all three problems adequately by accelerating the algorithm of the code MODCALIF to such an extent that a model calibration becomes feasible on a one-processor PC at first. Afterwards, the calibration of permeability, porosity, and transversal dispersivity is carried out in order to achieve the best agreement with the observed values. Finally, a stochastically founded approach for dispersivity is tested.

NUMERICAL ACCELERATION OF THE CODE MODCALIF

Previous works (Häfner & Boy, 2003 a, b) dealt with possibilities of the numerical acceleration of the code. So, the Peclet number criterion can be overcome (by means of the Front Limitation Algorithm – a special TVD Algorithm) and thus, a coarser grid can be used. The Courant criterion which strongly limits the time step is temporarily and locally suppressed (Courant-suppression) by temporarily allowing the full upwind weighting at critical points (i.e. in cells with Courant numbers Co >>1). As a third acceleration method the solution of the transport equation is limited to such partial domains of the grid which are expected to have a change in concentration $\Delta C > \varepsilon$ in the following time step.

For further acceleration the solver SAMG was involved in the code which led to an essential reduction in computing time by the factor 4-6. Similar to standard (geometric) multigrid, algebraic multigrid (AMG) combines the principles of smoothing and coarse grid correction to achieve rapid convergence. Rather than operating on a hierarchy of *grids*, however, AMG operates on a hierarchy of increasingly smaller *matrix equations*, constructed fully automatically, based merely on algebraic information which is explicitly or implicitly contained in the underlying matrices. However, as for geometric multigrid, AMG is not a fixed method but rather provides a methodology. The details of how the individual algorithmical components are finally constructed, strongly influence the resulting efficiency in terms of speed of convergence, memory requirement as well as robustness. In particular, for advection-dominant transport, standard Gauss-Seidel smoothing turned out to be only of a limited use. Instead, for the type of discretization used here, more robust ILU-type smoothers need to be employed.

The range of the acceleration methods resulted in the possibility to simulate each of the Saltpool experiments (phases 1-3 of case 1 and 2) on a one-processor PC (1.8 GHz) in about 13 hours. The same jobs lasted about 51 hours each with the PCG-Solver LINBCG after Press et al (1992). Similar Saltpool simulations with the program d^3f (Johannsen et al, 2002) took about 20 hours on a 16-Processor-PC-Cluster.

MODEL CALIBRATION

The initial parameters for permeability, porosity, and longitudinal/transversal dispersivity according to Oswald & Kinzelbach (2003) show a variation range with a mean value (initial parameter set). The parameters of tables 1 and 2 led to the outlet concentration course for case 1 (light) and case 2 (dense) shown in figure 1. The deviation from the observed values is considerable. Table 1 shows the sensitivities at the initial point of calibration as well as the calibrated parameters with those according to Johannsen et al (2002).

Table 1: Model calibration of Saltpool light experiment (case 1), parameters, model errors and sensitivities. Initial parameter set after Oswald & Kinzelbach (2003): $k=1\times10^{-9}$ m^2, $n=0.372$, $\alpha_{longitudinal} = 1.2\times10^{-3}$ m, $\alpha_{transversal} = 1.2\times10^{-4}$ m,

$$\left(\text{multiplicator} = \frac{\text{parameter value}}{\text{parameter value of the initial parameter set}} \right)$$

No.	Mean squared model error, % s.m.f.	Multiplicator for				Normalized sensitivity for			
		k	n	α_{long}	α_{trans}	k	n	α_{long}	α_{trans}
1	5.721×10^{-3}	1	1	1	1	0.688	1	0.027	0.096
2	3.821×10^{-3}	1.194	0.962	1	0.36	1	0.019	-	0.055
3	2.162×10^{-3}	1.131	0.993	1	0.50	0578	1	-	0.322
4	4.304×10^{-3}	1	1	1	1(stoch.)				
	Johannsen et al. (2002)	1.194	0.962	1	0.36	1	1	-	< 0.005
						(at the end of simulation)			

Table 2: Model calibration of Saltpool dense experiment (case 2), parameters, model errors and sensitivities.

No.	Mean squared model error, % s.m.f.	Multiplicator for				Normalized sensitivity for			
		k	n	α_{long}	α_{trans}	k	n	α_{long}	α_{trans}
1	36.78×10^{-3}	1	1	1	1	0.39	1	1.59×10^{-3}	0.424
2	15.03×10^{-3}	1.194	0.962	1	0.36				
3	1.774×10^{-3}	1.194	1	1	0.50	0.102	0.541	-	1
4	9.614×10^{-3}	1	1	1	1 (stoch)				
5	1.849×10^{-3}	1.131	0.993	1	0.50	0.211	0.426		1
	Johannsen et al. (2002)	1.194	0.962	1	0.36	0.47	1	-	0.27
						(at the end of simulation)			

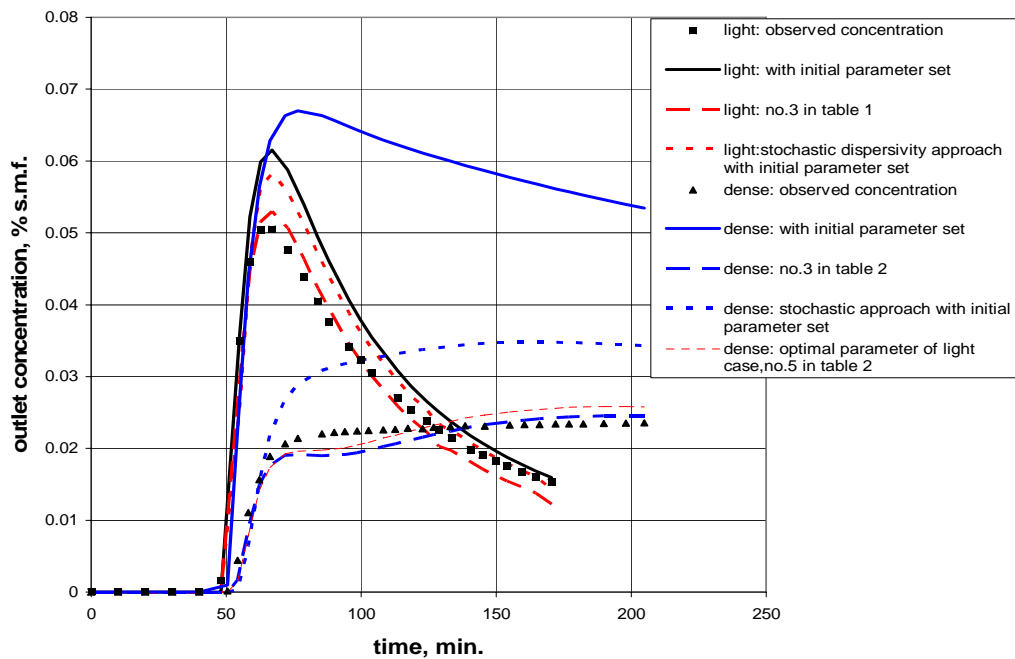Fig. 1 shows the simulated concentration courses with calibrated parameters.

Fig.1 Outlet concentration of Saltpool experiments case 1 (light) and case 2 (dense), observed values, initial parameter set after Oswald & Kinzelbach (2003) and MODCALIF calibration results.

In Figure 2 a diagonal vertical cross-section of concentrations at the end of the phase 2 are shown, compared with the observed values. The agreement seems to be satisfactory.

STOCHASTIC DISPERSIVITY APPROACH

For a Gaussian-distributed velocity in one-dimensional transport Rösler & Schwan (1986) showed that the longitudinal dispersivity is in proportion to the flow distance. The simulation of the experiments without model calibration was carried out with this approach which is very similar to the stochastic interpretation of dispersion according to Dagan (1989). In the simulation the maximum flow distance in each of the phases 1-2 corresponds to the distance of the source (centrally at the bottom of the test box) from the outlet openings (in the upper corners of the box). In phase 3 the maximum flow distance corresponds to the diagonal distance of entry and outlet openings. Figure 1 shows the results.
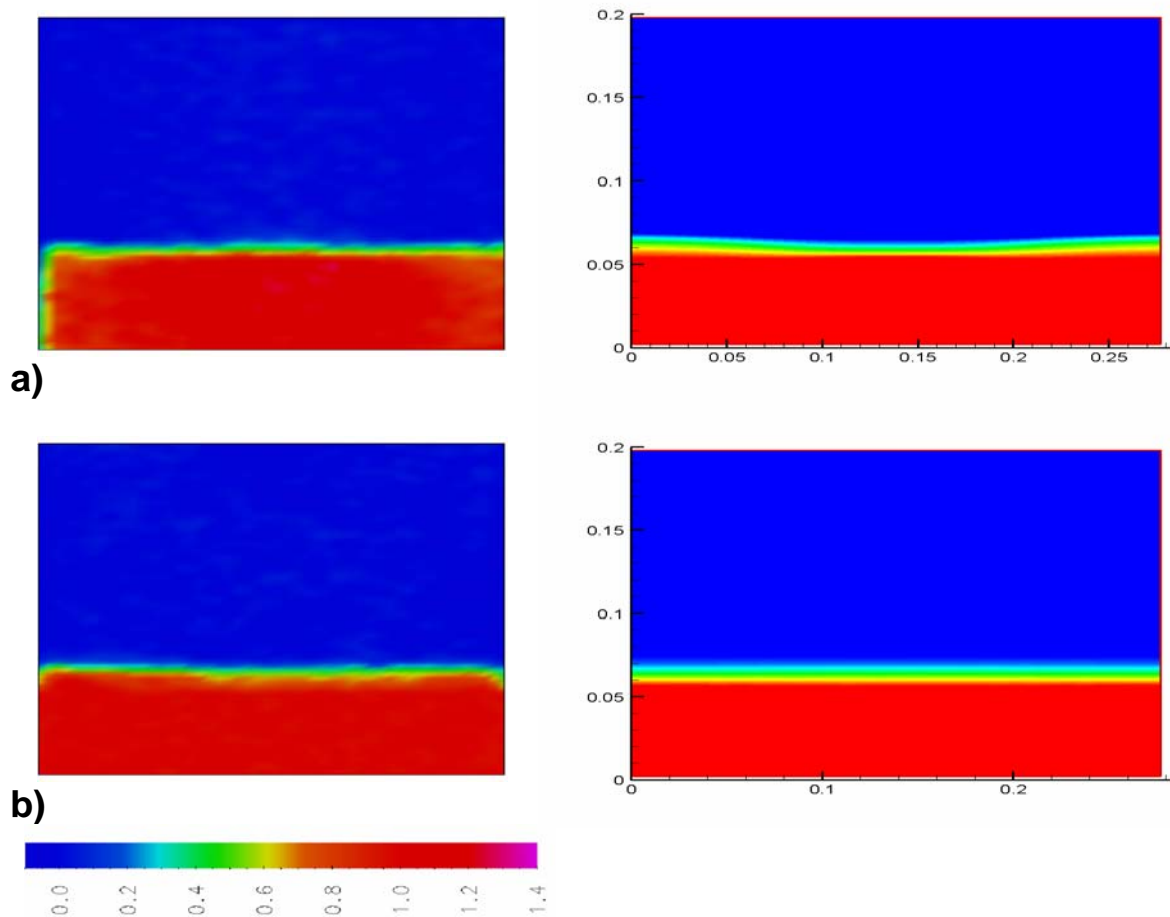
Fig. 2 Relative concentrations in a vertical diagonal cross-section at the end of phase 2. Left: measured ,after Oswald (2003), Right: simulated with calibrated parameters after tables 1, 2.
a) case 1-light, after 43.46 min.   **b)** case 2-dense, after 44.93 min.

CONCLUSIONS

The simulation of the Saltpool experiments with MODCALIF shows that good results can quickly be achieved also with common PCs. Without calibration the stochastic dispersivity approach leads to concentrations which come nearer to the observed values.

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