Experimental and Numerical Investigation of Macrodispersion of Density-Dependent Transport in Stochastically Heterogeneous Media: Effects of Boundary Conditions and High Concentrations

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ABSTRACT

Experiments of macrodispersion in density-dependent flow within stochastic realizations of a heterogeneous medium are being performed in the new 10 by 0.1 by 1.2m large Plexiglas tank at the hydraulic laboratory of the University of Kassel. Objective of the ongoing long-term study is the analysis of the effects of the stochastic properties of the porous medium on the steady-state macrodispersion. Several experiments with saltwater concentrations ranging from $c_0 = 250$ (fresh water) to $c_0 = 100000$ ppm and two inflow velocities of $u = 1$ and $u = 4$ m/day each are carried out for the hydrodynamically stable case of saltwater injection underneath a layer of fresh water for two anisotropically packed sand structures with different variances and correlation lengths for the permeability variations. Depending on the flow velocities, steady-state conditions for the macrodispersive transport with the saltwater plume extending over the whole length of the tank are reached after about two weeks.

For calibration and validation purposes the experiments are accompanied by numerical simulations using the SUTRA density-dependent flow and transport model. To properly mimic the associated macrodispersion experiment it was found that the boundary conditions (BC) for the pressure $p$ and, even more so, for the concentration $c$ in the outflow have to be correctly chosen in the SUTRA code. If one uses the natural (free) boundary condition for the concentration at the outlet, the saltwater plume sinks stronger and has a smaller dispersion width than for the modelled plume that arises from the use of the Dirichlet concentration boundary condition $C = C_{mix}$, where $C_{mix}$ is the mixing concentration of the outflow and is about half of the input concentration $c_0$ at the saltwater inlet. As is to be expected, these differences increase with increasing saltwater concentration, i.e. increasing density contrast. For the second BC-case the numerical models are also much more in agreement with the experimental results. Since the Dirichlet concentration BC acts only for inflow into the model, these results show that there must be a small amount of return flow of the mixing saltwater from the outflow chamber back into the tank.

Both experiments and numerical models indicate for the same concentration contrast $c_0$ a larger sinking of the mixing layer with decreasing inflow velocity and, at the same time, a widening of the former, i.e. an apparent increase of the lateral dispersion coefficient $D_T$. At present it is still at debate whether this, obviously, contradictory behaviour with regard to the stability of the saline plume is due to the particular local vertical permeability distribution of the tank at the positions of the sampling section, which appear to have a significant impact on the apparent lateral dispersion there, or that it is a consequence of an imbalance of molecular and mechanical dispersion. This peculiar situation is particularly prevalent for the high saltwater concentration experiment with $C_0 = 100000$ ppm, where one notes an anomalous strong increase of the lateral dispersion for the low flow velocity case $u = 1$ m/day. Whether this hints of some non-Fickian dispersion phenomenon, as it has been postulated by some authors for very high saline concentrations, or that is just due to the particular stochastic realization of the present tank-packing, is being investigated further.

1. INTRODUCTION

Variable density flow and transport in porous media occurs in many facets in groundwater hydrology such as, for example, (1) seawater intrusion in coastal aquifers [Bear et al., 1999]; (2) saltwater upconing in formation aquifers [Voss and Koch, 2001]; (3) vertical seepage of brackish water from open ocean canals [Koch and Zhang, 1998]; (4) movement of brine solutions in salt domes that have been targeted as possible nuclear waste repositories [Herbert et al., 1988]; (5) infiltration of dense aqueous (miscible) or non-aqueous (immiscible) phase liquids [Kimmel and Braids, 1980], to name a few. From a physics point of view the peculiarity and intricacy of variable
density flow and transport stems from the fact that, due to the coupling of flow and transport, buoyancy effects are introduced in the flow field which, in addition to the regular head gradients, may constitute a dominant driving force for the flow. Depending on the density stratification, stable (as in the cases (1) and (2) above) or unstable flow pattern (fingers) (as in the cases (3) and (5) above) of the solute plume may then develop.

Since the first studies of miscible water-oil displacement in secondary petroleum recovery [Perrine, 1963] and the subsequent theoretical studies of Wooding [1962, 1969] on the onset and evolution of unstable modes and fingers for an unstable density stratification has found particular interest during the last few decades, both experimentally [e.g. Schincariol and Schwartz, 1990; Oostrom et al. 1992] and through numerical simulations in homogeneous [Koch, 1992; 1993; Koch and Zhang, 1992] and heterogeneous [Koch, 1994] porous media structures. Strong density effects with the development of fingers were observed in these studies for already moderate solute concentrations, indicating the need of taking density effects into account in the practical modeling of such flow and transport situations. However, as discussed in detail by Voss and Koch [2001], the extra computational efforts required for full density-dependent transport simulations, when compared with those for the uncoupled tracer problem, may in many practical situations be prohibitive, particularly for a heterogeneous aquifer structure. Therefore, a need exists for some more “basic” approaches to describe the salient physical phenomena arising in density-dependent flow and transport processes.

One way of approaching this problem is to somehow relate the apparent dispersion coefficients $D_L$ and $D_T$ to the density contrast across the fluid interface between the solute plume and the fresh water. For a hydrodynamically stable configuration (denser fluid below) one expects a decrease of the dispersion with increasing density, while for an unstable layering (denser fluid above) the opposite holds. This has indeed been shown to be the case experimentally by Kobus and Spitz [1985] and theoretically through a boundary analysis of the shearing mixing layer by Thiele [1997]. However, in both studies it is demonstrated that the density effects on the apparent dispersion can only be observed in the mechanical dispersion regime, i.e. when the Peclet number is significantly larger than unity. Moreover, in the tank experiments of Kobus and Spitz [1985], a reduction of the width of the mixing zone, i.e. a decrease of the lateral dispersion ($D_L$) with increasing density contrast, is obtained only for a sand packing with a non-uniform grain distribution. This indicates that the density-dependent dispersion processes must act on a larger-than-the-normal pore-size scale, i.e. scale-dependent macrodispersion prevails. It follows that this phenomenon must also play an important role in variable density flow [Welty and Gelhar, 1991], as it is accepted now to be the case for regular tracer flow and transport [Gelhar, 1993].

The next logical step is then to use a full stochastic approach for the description of macrodispersion in variable density flow and transport in heterogeneous porous media, using the now well-known methods of stochastic theory [cf. Gelhar, 1993]. This is the ultimate objective of this ongoing study, namely the experimental verification of some of the theoretical predictions for the effective macrodispersion that may occur in a stochastically packed heterogeneous sand structure in a laboratory tank. Here we report on first results of such tank experiments for the dynamically stable case of saltwater injection of various concentrations and seepage velocities underneath a layer of fresh water.

2. TANK EXPERIMENTS

2.1 Experimental setup and program

The new Plexiglas tank of the hydraulic laboratory of the University of Kassel is $x = 10$ m long, $y = 0.1$ m wide, and $z = 1.2$ m high. Inflow and outflow chambers are attached to the two ends of the tank, separated from the sandpack by a permeable fleece. The inlet chamber itself is separated in the middle into two independent sub-chambers by a horizontal plastic plate which protrudes about 0.25 m into the tank, thus providing an initial interface between the inflows from the two sub-chambers before these are able to mix with each other in the tank (Figure 1).

For the purpose of the present analysis of macrodispersion for a stable fluid stratification the upper inlet chamber is attached to a supply tank of distilled and de-ionized water and the lower inlet chamber to a tank of a prepared solution of given concentration $C_0$ of chemically pure NaCl in distilled and de-ionized water. The horizontal hydraulic gradient across the tank that is driving both the fresh- and the saltwater flow is adjusted by raising or lowering the two small inflow/overflow containers with respect to the outflow/overflow container. Determination of in situ concentration is done by taking fluid samples at about 126 hollow needle ports placed along 6 vertical transects positioned at the horizontal locations shown in Figure 1, measuring their electric conductivity, and relating them to previously established conductivity/concentration calibration curves.
In view of the objectives of this ongoing study, namely, the analysis of the effects of a stochastic heterogeneous porous medium on the macrodispersion in variable density flow, the tank is packed following a computer-generated stochastic realization of a random medium whose properties, following the laws of the well-known stochastic theory [c.f. Gelhar, 1993], is fully characterized by the mean \( \bar{Y} \), variance \( \sigma^2 \), and correlation lengths \( \lambda_x \), \( \lambda_y \), and \( \lambda_z \) (where for a 3D isotropic medium \( \lambda_x = \lambda_y = \lambda_z \)) of the stationary Gaussian process \( Y = ln(k) \) of the permeability distribution of \( k \). At the time of this writing experiments with a tank packing with mean \( \bar{Y} = ln(k) \) of the present tank packing with the positions of the six observation ports indicated. Note the vertical exaggeration of the tank height.

**Figure 1:** Design and setup of tank experiment.

As part of this long-term ongoing study on macrodispersion in density-dependent flow, a series of experiments for the stable stratification case has been carried out. The two parameters varied in these experiments are (1) the concentration \( C_0 \) of the saltwater (NaCl-solution), and (2) the inflow velocity \( u \) of both the fresh and the

**Figure 2:** Stochastic realization of permeability \( k \) \( [cm^2] \) of the present tank packing with the positions of the six sampling ports indicated. Note the vertical exaggeration of the tank height.
saltwater. At present four experiments with $C_0 = 250$ ppm (pure tracer), $5000$ ppm, $35000$ ppm (seawater) and $100000$ ppm were run, each with two different inflow (seepage) velocities $u$, namely $u = 1 \text{ m/day}$ and $u = 4 \text{ m/day}$.

The experiments of Koch and Starke [2001], which were run only up to a saltwater concentration of $35000$ ppm and, more importantly, for constant inflow boundary conditions, i.e. attempts were made to keep the fresh and saltwater inflow rates equal throughout the time-span of one experiment --- up to three weeks before steady state is reached which was very difficult to achieve practically, since the heights of the inlet overflow chambers has to be adjusted meticulously, with the effect of changing tremendously the pressure equilibrium of fresh and saltwater interface. On the other hand, the present experiments are performed with constant head boundary conditions (BC) imposed at the inflow and outflow chambers of the tank. As will be shown in a later section, apart from being experimentally better to sustain, are these Dirichlet BC’s also easier to implement into the numerical model SUTRA.

### 2.2 Experimental results

Figures 3 and 4 summarize the most salient results of all the tank experiments run up-to-date. Figure 3 shows the measured concentration ratios $C/C_0$ over the depth of the tank at port columns 27 and 47 (see Figure 1 for horizontal locations), whereas Figure 4 depicts the same data in a reshuffled combination to allow for the analysis of various physical aspects of the study phenomenon. With respect to the latter, answers to two questions are of particular interest: (1) What is the effect of increasing concentration contrast on the dispersion process? (2) What is the effect of the inflow velocity $u$ on the latter? The positions and the forms of the $C/C_0$-curves in Figures 3 and 4 provide partial answers, as they can be related to the location of the center and of the width of the mixture zone between the fresh- and the saltwater layer. With respect to the two questions above the following observations can be made from Figure 3 and 4:

For the sampling port C27, located in the middle section of the tank, one notes a systematic sinking of the plateau of the $C/C_0$-curve with increasing concentration $C_0$ up to $C_0 = 35000$ ppm for both inflow velocities $u$. However, for the high concentration case $C_0 = 100000$ ppm an anomalous situation appears to be prevalent, with the plume-plateau located higher than for $C_0 = 35000$ ppm. Similar behaviours of the plumes are found for the other sampling ports C33, C37 and C43 located further downstream the tank. However, as can be recognized from Figure 3 a peculiar situation arises at the last sampling port C47 which is located about 0.6 m from the outflow chamber of the tank. Here a double S-shape like $C/C_0$-curve is observed for the experiment with $C_0 = 100000$ ppm and low inflow velocity $u = 1 \text{ m/day}$. For the experiment with the larger inflow velocity $u = 4 \text{ m/day}$, however, the situation reverses back to normal. As it turns out, and could only be vindicated by the SUTRA numerical experiments, the strange behaviour for the former experiment is due to a small amount of density-triggered return flow of the mixing solution in the outflow chamber which at steady-state has always a concentration of $C_{\text{mix}}$ equal to $C_{\text{mix}} = C_0/2$. For the larger flow velocity $u = 4 \text{ m/day}$, on the other hand, the horizontal flow gradient is large enough to prevail over small density-induced reverse local flows from the mixing chamber into the tank.

Figure 4 displays in a more illustrative manner the effects of the inflow velocity $u$ on the concentration profiles. For both the experiments with $C_0 = 5000$ ppm and $C_0 = 35000$ ppm one notices a larger sinking of the plume center for $u = 1 \text{ m/day}$ than for $u = 4 \text{ m/day}$, i.e. the density effect is the more prominent, the smaller the transport velocity. Thus, if one assumes the classical relationship for the transverse mechanical dispersion $D_T = \alpha_T u$ [Bear, 1979], with $\alpha_T$ the transverse dispersivity, this result provides evidence that dispersion has a stabilizing effect on the negatively buoyant plume. However, for the $C_0 = 100000$ ppm experiment, this situation is reversed at the sampling port C37 shown (and also at the other port columns in the interior of the tank) and mixed at the last sampling port C47, with the aforementioned double S-shape like concentration profile for $u = 1 \text{ m/day}$. At the present time it can only be surmised that a different (nonlinear) dispersion mechanism may act at such high saline concentrations, as it has already been witnessed in other author’s studies of this kind [Hassanizadeh and Leijnse, 1995; Schotting, 1999].

A more detailed analysis of the macroscopic dispersion originates from the analysis of the widths $\sigma$ of the mixing zones of the fresh and saltwater layers for the various experimental situations. The latter are measured approximately from the difference of the $z$-locations for the $C/C_0 = 0.16$ and $C/C_0 = 0.84$ values on the $C/C_0$-curves, respectively, and are illustrated in different manners in Figures 5 and 6. From Figure 5 one observes, other than for the case $C_0 = 100000$ ppm and $u = 1 \text{ m/day}$, that there is no systematic change of $\sigma$ with the horizontal position $x$. This is contrary to what one expects theoretically for shear flow in a homogeneous porous medium where the dispersion width $\sigma$ can be shown to behave as $\sigma \sim \left(2\alpha_{T, x}\right)^{0.5}$ [Thiele, 1997]. There is evidence that the dispersion width $\sigma$ at a particular
x is somehow related to the local permeability distribution of the tank there and appears to be larger in sections where the permeability is reduced (see Figure 2). In fact, Figure 6 reveals that the dispersion width $\sigma$ is larger in the middle and rear sections of the tank for the smaller velocity value $u = 1$ m/day than for $u = 4$ m/day. If one assumes that the effective dispersion increases the stability of the plume, this result appears to be somewhat contrary to the previous findings in Figure 4 from which an increased stability (less sinking) of the saline layer was deduced. for the larger velocity $u = 4$ m/day than for $u = 1$ m/day.

Finally Figure 6 shows also that, particularly, for the velocity $u = 4$ m/day, the dispersion width $\sigma$, i.e. the transversal dispersion coefficient $D_T$, is increasing with increasing saline concentration, i.e. density contrast $\Delta \rho$. This is contrary of what has been found for stable density stratification, as well in the tank experiments of Kobus and Spitz [1985] as theoretically by Thiele [1997], both of which obtained a decrease of $D_T$ when $\Delta \rho$ augments. This, however, only when the mechanical dispersion $D_T^{mech}$ is much larger than the molecular dispersion $D_m$, which is the case for Peclet numbers $Pe = u*d/D_m \gg 1$ [Bear, 1979]. The average grain size $d$ for the present tank sand packing is $d = 0.8$ mm. This results in $Pe$-numbers $Pe = 7$ and $Pe = 28$ for the two inflow velocities $u = 1$ and $4$ m/day, respectively, which means that hydrodynamic dispersion may not yet play an important role in our experiments, unlike in those of Kobus and Spitz [1985] which were run with $Pe$-numbers ranging from $Pe = 1500$ to $Pe = 3000$. Therefore, the apparent contradictions in the interplay of the effective dispersion and the density effect in the present experiments, as deduced from Figures 5 and 6, may also be related to this peculiarly prevailing dispersion regime.
Figure 4: Effects of inflow velocities on the plume plateaus for the various experiments with concentrations $C_0 = 5000$, 35000 and 100000 ppm (from top to bottom panels) at port columns 37 and 47.
3. NUMERICAL SIMULATIONS
3.1 Description and setup of the model

In parallel with the laboratory tank experiments numerical simulations of the density-dependent flow and transport configuration, as depicted in Figure 2, were performed, using the 2D density-dependent flow and transport finite element model SUTRA [Voss, 1984]. The mathematical equations solved by SUTRA are the (a) groundwater flow for the piezometric pressure \( p \) and (b) the advection-dispersion transport equation for the solute concentration, both of which are coupled through (c) an equation of state between density and solute concentration \( C \) [e.g. Bear, 1979]. However, since the original SUTRA code does not include viscosity dependency of the fluid on the concentration, the code was modified here to that regard and simulations with variable viscosity were also performed.
The SUTRA model grid was set up to mimic the x-z cross-sectional geometry of the tank. To resolve the stochastic random permeability field in the tank (Figure 2), each sand block was represented numerically by 8 x 4 elements, resulting in a total of \( n_x \times n_y = 392 \times 98 = 38416 \) elements. In extension of the earlier studies of Koch and Starke [2001], where mainly only deterministic models of the experimentally given flow and transport characteristics, including the experimental sandpack permeabilities of the tank, were carried out, in the following results of numerous stochastic Monte Carlo simulations are presented, allowing for a better grasp of the physics of the problem at hand.

As will be shown in the present section, the choice of the inflow, and even more so, the outflow Dirichlet boundary conditions (BC’s) for the hydrostatic pressure \( p \) plays a dominant role on the modeled physics of the density-dependent flow and transport problem. Whereas in the earlier SUTRA simulations of Koch and Starke [2001], the outflow BC for \( p \) was set to be equal to the initially set outflow fresh water head (BC0), giving rise to some discrepancy in the experimental and modeled plume positions, recently we have used a Dirichlet BC for \( p \) that is more consistent with the pressure distribution of the homogenously mixed fresh and saltwater (through a stirrer, as shown in Figure 1) in the outflow chamber at steady state conditions. Measurements showed that the mixing concentration \( C_{\text{mix}} \), is about half of the input concentration \( C_i \) at the saltwater inlet so that this pressure BC (denoted as BC1 in the following) at the outflow boundary varies with depth \( z \) as \( p_{BC} = \rho \left(C_{\text{mix}}\right) \sigma g \, z \), where \( \rho \left(C_{\text{mix}}\right) \) is the density at that concentration \( C_{\text{mix}} \), as evaluated through a standard equation of state.

### 3.2 Results of deterministic models and comparison with experiments

Figure 7 shows SUTRA-modeled concentration profiles (using the real tank-pack permeability distribution) at sampling ports C37 and C47 for the different tank experiments with varying concentrations \( C_i \) and inflow velocities \( u \), using either the pressure boundary condition BC0 (fresh water head) or BC1 (mixed saltwater head) at the outflow boundary. The transversal dispersivity used in all these deterministic models is \( \alpha_f = 1.9*10^{-3} \, \text{m} \), which was shown through several trial and error runs to be the best to mimic the observed dispersion zones of the previous section.

The most striking feature of Figure 7 is the tremendous influence of the outflow boundary condition, namely, on the plateau levels of the fresh-saltwater interface and the mixing zones, such that the latter are consistently located much higher for the new BC1 than for the old BC0 pressure boundary condition. These differences are particularly pronounced at sampling ports C47, close to the rear end of the tank and, expectedly, for the large saline concentrations \( C_i = 35000 \, \text{ppm} \) and, even more so, for 100000 ppm. In any case, since the results for BC1 simulations are also much more in agreement with the positions of the observed experimental plateau levels in Figures 3 and 4, this provides sufficient evidence that the physics of the present density-dependent transport problem is much better modeled by using the BC1 boundary condition. Therefore, the following discussion will refer only to the results of these BC1 simulations.

Similar to the analysis of the experimental results, the variations of both the vertical location of the plume center and of the width of the dispersion zone as a function of the saline concentration \( C_i \) and of the inflow velocity \( u \) are of particular interest. With respect to the former, Figure 7 shows that, naturally, the plume center sinks with increasing concentration, regardless of the inflow velocity \( u \). Moreover, the effect of the latter is such, that the smaller \( u = 1 \, \text{m/day} \) results in a larger sinking of the plume center than the velocity \( u = 4 \, \text{m/day} \). This, surprisingly, is in full agreement with the experimental results (Figure 4), providing evidence, now also from the numerical model, that dispersion has a stabilizing effect on the negatively buoyant plume.

Regarding the width \( \sigma \) of the dispersive mixing zone, the numerical models appear to show, albeit to a very small degree, a similar trend as the experiments, namely, that \( \sigma \) is larger in the middle and rear sections of the tank for the smaller velocity value \( u = 1 \, \text{m/day} \) than for \( u = 4 \, \text{m/day} \), facing us with the similar problem to explain a somewhat contradictory result, since the stability of the plume should go in parallel with less sinking of its center and a larger dispersion width. However, as argued in Section 2.2, a possible reason for this apparent discrepancy may be searched in the particular local vertical permeability distributions of the tank at the positions of the sampling sections, which appear to have a significant impact on the apparent lateral dispersion there. To further analyze this phenomenon, numerical (Monte-Carlo) simulations of the macrodispersion of the density-dependent transport problem, using different stochastic realizations of a random medium within the tank are, presently being carried out and will be reported on in the near future.
**Figure 7:** SUTRA-modeled concentration distributions at sampling ports C37 and C47 for the different tank experiments with varying concentrations $C_0$ and inflow velocities $u$ using pressure boundary conditions BC0 (fresh water head) and BC1 (mixed saltwater head) at the outflow boundary. The transversal dispersivity used is $a_T = 1.9 \times 10^3$ m.

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