LABORATORY EXPERIMENTS AND MONTE CARLO SIMULATIONS TO VALIDATE A STOCHASTIC THEORY OF DENSITY-DEPENDENT MACRODISPERSION

BETTINA STARKE AND MANFRED KOCH[1]

[1]*Department of Geotechnology and Geohydraulics, University of Kassel, Kurt-Wolters Str. 3, D-34119 Kassel, Germany*

ABSTRACT

Monte Carlo (MC) simulations of density-dependent flow and transport have been performed to calibrate and validate tank experiments as well as a stochastic theory of macrodispersion in heterogeneous medium. Final objective of this study is to quantify the effects of the stochastics of the porous medium on lateral macrodispersion. 2D (x,y) tank experiments of stably stratified density-dependent flow and transport are carried out for three stochastic, anisotropically packed sand structures with different, variance σ^2_{lnk}, and horizontal and vertical correlation lengths λ_x , λ_y for the permeability variations. For each flow and transport experiment, a large number of MC-simulations with the FE-program SUTRA, using stochastic realizations of the corresponding statistical family, are executed. From moment analyses and laterals widths of the simulated saltwater plumes, variances $\sigma^2_c(x)$ of the lateral dispersion and, subsequently, expectation values for the transversal dispersivity $E(A_T)$ are calculated. To validate a theoretical formula proposed by Welty et al. (2003) for the transversal macrodispersivity A_T, the sets of experimental as well as numerical results for A_T are subject to a multiple linear regression analysis. A very good agreement for the tracer results and a reasonable good agreement for the density-dependent ones with the analytical formula is observed. Finally, the sensitivity of A_T to various medium and flow parameters is investigated. Besides to the choice of the pressure BC at the tank boundaries, A_T, expectedly, is rather sensitive to the heterogeneity $H \sim \sigma_{lnk}^2 * \lambda_x$ of the porous medium.

1. INTRODUCTION

Extensive research on the dispersion of a dissolved water substance began five decades ago with the fundamental work of Scheiddegger (1958). Due to the complexity of the flow and transport processes, an accurate mathematical description at the microscopic pore level is still lacking. One way out of this dilemma has been the introduction of a dispersion coefficient D that somewhat foregoes the details of the physics occurring at the pore level. D is a second order tensor and depends both on the characteristics of the fluid and, as revealed by the more recent theories of stochastic hydrology (Gelhar and Axness, 1983; Gelhar, 1993), on the heterogeneity of the porous medium. Moreover, experimental (Schincariol and Schwartz, 1990; Schotting et al., 1999), theoretical (Thiele, 1997) and numerical investigations (Koch; 1992; 1993; Koch and Zhang, 1992) showed that this model, since still being based on the classical Fick's law, does not hold anymore for higher concentrations.

Scenarios of density-dependent flow and transport arise in many areas of groundwater hydrology, e.g. seawater intrusion in costal aquifers (Koch and Zhang, 1998), saltwater upconing in freshwater formations (Voss and Koch, 2001) and, generally, the transport of pollutants with different density (Koch and Zhang, 1992). Depending on the density stratification one distinguishes between the stable case, where the denser fluid is flowing below the less dense one, and the unstable case, with the denser fluid above the lighter other. The unstable case experiences (Rayleigh-Taylor) instabilities already for small density contrasts, leading to so-called “fingers”, that penetrate slowly into the lower layer (e.g. Koch 1992, 1993, 1994; Koch and Zhang, 1992; 1998; Schincariol and Schwartz). A widening of the dispersive interface is observed with increasing density gradients in this case, whereas the opposite for the stable case (Spitz, 1985; Thiele, 1997).

Most of the studies mentioned pertain to density-dependent flow and transport in homogeneous porous medium. However with the advent of the stochastic theory of macrodispersion, mostly of tracer flow, in heterogeneous media (Gelhar and Axness, 1983, Gelhar, 1993), there is need to establish a verified knowledge about density-induced flow and transport in stochastically heterogeneous formations. The next logical step is then to use a full stochastic approach for the description of macrodispersion in variable density flow in heterogeneous porous media, using the now well-known methods of stochastic theory. First steps along these lines have been made by Welty et al. (2003) and the ultimate objective of the present, still ongoing study is, namely, the experimental verification of some of their theoretical predictions for the effective macrodispersion in a stochastically packed heterogeneous sand structure within a laboratory tank. Here we report on some newest results of tank experiments (cf. Starke, 2005) and Monte Carlo simulations regarding the coupled effects of fluid flow/density and medium heterogeneity on the macrodispersion, namely, the lateral dispersivity and, eventually, reconciling it with the ideas of stochastic theory.

2. TANK EXPERIMENTS

2.1 Stochastic packing of the tank

To verify the stochastic models experimental studies in a 9.8 m long, 1.225 m high and 0.10 m wide model tank at the University of Kassel were carried out (Fig. 1). With these dimensions stochastically "homogeneous" conditions should be achieved, i.e. the porous medium is much larger than its heterogeneity-scale, as measured by its correlation length.

As a model configuration layered horizontal flow ($u = u_x$) is generated through an intake of fresh (degassed) water flow in the upper half of the tank and of saline tracer of NaCl with varying concentration $c = c_0$ in the lower half one. To control the flow rate u, the heights of the overflow containers at the tank inlet and outlet are manually adjusted. For the measurement of the concentrations tiny amounts of fluid are extracted by a medical syringe at 126 sample ports drilled in 6 vertical planes across the horizontal extensions of the tank and its electrical conductivity determined. With increasing flow length the tracer front disperses horizontally and vertically. For $t \rightarrow \infty$ a stationary concentration distribution adjusts itself. A lateral mixing boundary of width B(x) between the two fluid sections forms which will be used to determine the lateral macrodispersivity A_T.

The sand pack was generated beforehand by means of the TBM random number generator

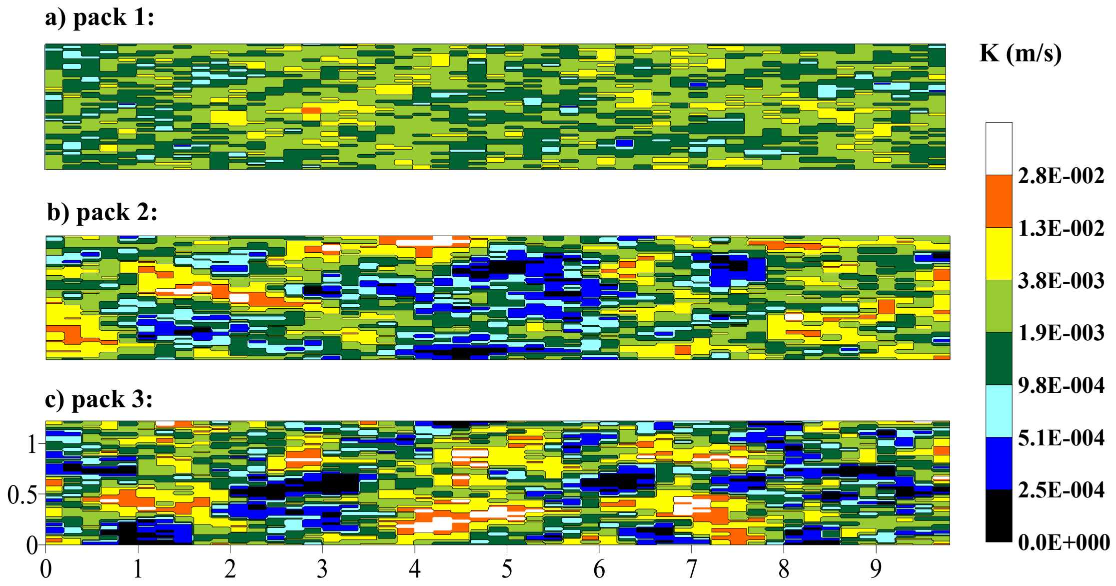

FIGURE 1: Stochastic realizations of hydraulic conductivity field Y= ln K for 3 tank packs with mean $Y_g = \ln(K_g) = -13.25$ and, a) pack 1: $\sigma_Y^2 = 0.25$, $\lambda_x = 0.2$ m, $\lambda_y = 0.05$ m, b) pack 2: $\sigma_Y^2 = 1.00$, $\lambda_x = 0.4$ m, $\lambda_y = 0.10$ m and, c) pack 3: $\sigma_Y^2 = 1.50$, $\lambda_x = 0.3$ m, $\lambda_y = 0.075$ m.

(Tompson et al., 1989) as a realization of a stationary log-normally distributed hydraulic conductivity field Y = ln K, with given mean Y_g, variance σ_Y^2, and correlation lengths λ_x, λ_y. In order to fulfil the conditions of ergodicity, the length of the maximal transport distance should amount to about ten times λ_x which, given the values in the caption of Fig.1 where the three sand pack realizations are shown is, in principle, the case.

2.2 Experimental program and results

For each of the three stochastically packed sand structures (Fig. 1) a series of controlled experiments tank experiments has been carried out with different concentrations c_o of the lower, dense fluid, that range from $c_o = 250$ to $c_o = 100000$ ppm, and three different inflow velocities u = 1, 4 and 8 m/day, respectively. After reaching steady state (depending on the flow velocity, this can vary from 3 to 14 days), the vertical concentration profiles c(y) at the 6 vertical columns are determined and graphed (see Starke, 2005, for details). The transversal dispersivity A_T is then calculated as $A_T = 0.5 * d\sigma_c^2(x)/dx$, i.e. through simple linear regression of the spatial (2D) moments $\sigma_c^2(x) = (B(x)/2)^2$ (with B(x) the mixing width of the vertical concentration distribution along the distance x from the tank inlet and which is determined from the those differences in the vertical locations where the normalized concentration are 0.16 and 0.84, respectively). Fig. 2 depicts $\sigma_c^2(x)$ for two sand packs and various concentrations c_o. One can observe that the boundaries of the concentration plumes are varying in an undulatory way across the horizontal extension of the tank, attributable possibly to non-ergodic effects. We also noticed that the wavelengths of these undulations are proportional to the correlation lengths λ_x, but neither of c_o, nor of the flow velocity u.

Fig. 3 shows some results obtained for A_T as functions of u, c_0 and the heterogeneity factor $H \sim \sigma_{lnk}^2 * \lambda_x$ (additional results are presented in Starke (2005)). One notes a nonlinear

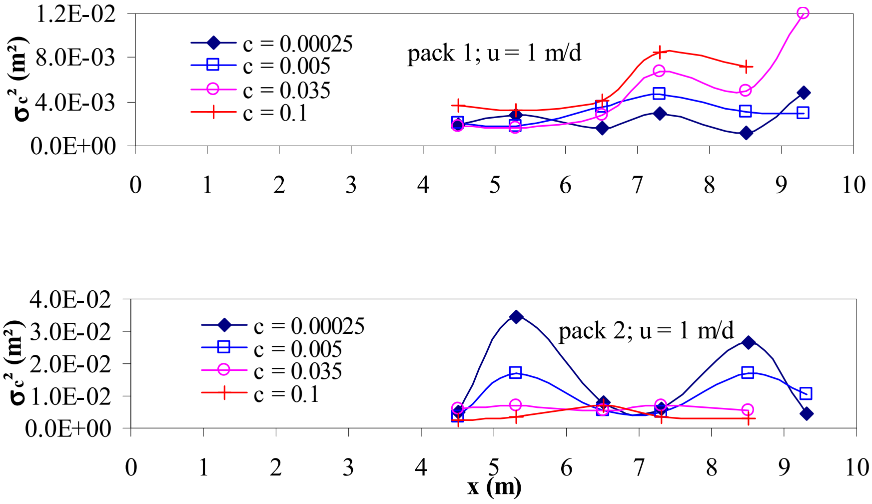

FIGURE 2: Spatial variances σ_c^2 of the concentration distribution as a function of the displacement distance for pack 1 (above) and pack 2 (below) and seepage velocity u = 1 m/d.

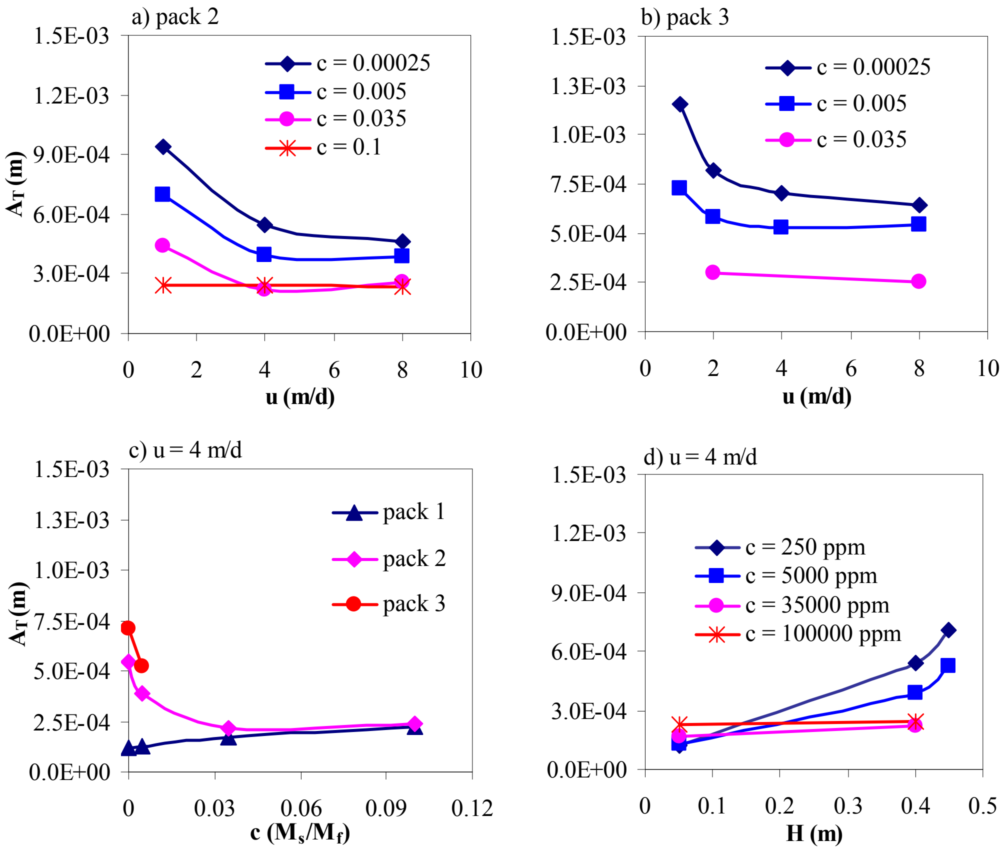

FIGURE 3. Experimental results for A_T as a function of velocity u for pack 2 (a), pack 3 (b), and as function of concentration (c), and the heterogeneity H (d).

decrease of A_T with increasing seepage velocity, until an asymptotic value for large u is reached. A_T is also increasing with the heterogeneity H of the porous medium (Fig. 3d), but is decreasing with the density difference Δc between the two fluids (Fig. 3c).

3. MONTE CARLO SIMULATIONS

For each tank experiment a number of MC-simulations with stochastic (TBM) realizations that are representative of the statistical family of the sand pack (variance σ_Y^2, correlation lengths λ_x, λ_y) are performed with the SUTRA FE-flow and transport model (Voss, 2003). Similar to the analyses of the experiments, spatial variances $\sigma^2_c(x)$ are evaluated from the concentration profiles, and an expectation value $E(A_T)$ for the transversal macrodispersivity is computed from the set of MC-simulations that mimics the particular medium family and given flow conditions. Fig. 4 depicts the cumulative results obtained with 100 MC-runs for the stochastics of sand pack 1 and tracer flow (c_0=250ppm, i.e. density-independent) of u=4m/d. One observes that the experimental results are located well within the "+- one" standard deviation band s (~68% confidence interval) of the computed $E(\sigma^2_c)$.

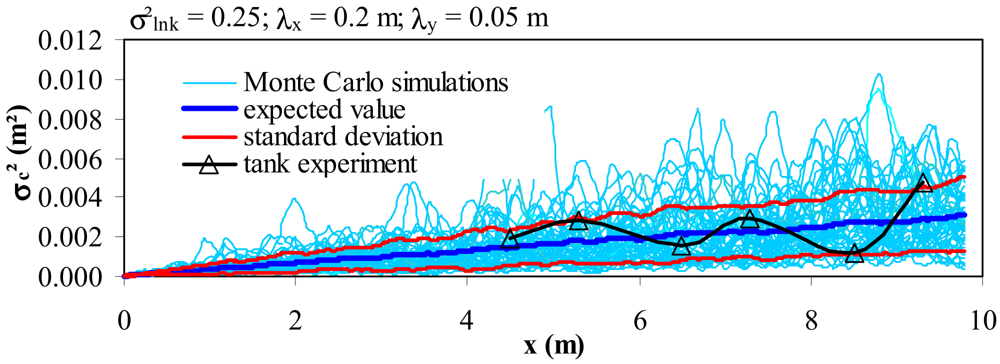

FIGURE 4: Ensemble $\sigma_c^2(x)$ for 100 MC- simulations with expectation value $E(\sigma_c^2)$, "+- one standard-deviation" band and the corresponding tank experiment for sand pack 1.

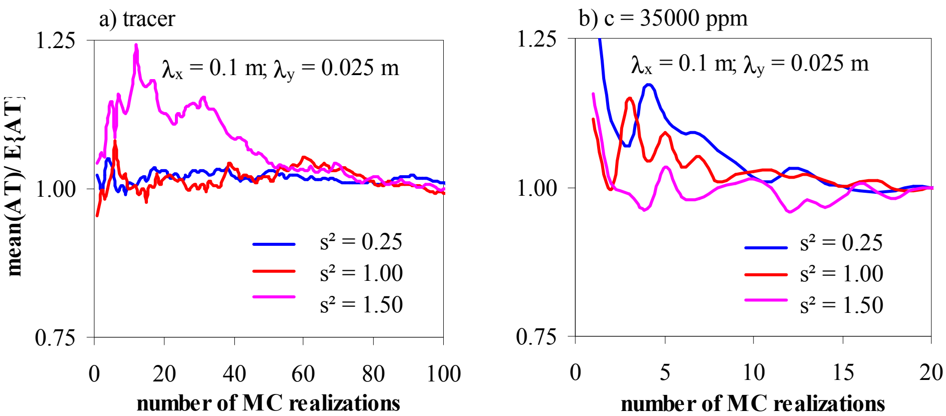

FIGURE 5: Normalized mean of A_T as a function of the number of MC-realizations for a) density- independent (tracer) case and, b) density-dependent case.

Fig. 5 shows $E(A_T)$ as a function of the number N of MC-simulations. Interestingly, convergence is reached earlier for the density-dependent (N~30) than for the tracer cases (N~100), showing the stabilizing effects of the former. Fig. 6 illustrates the MC-computed $E(A_T)$ values as a function of the porous-medium stochastics (σ^2_{lnk}, λ_x , λ_y) and of the flow and transport parameters (u, c_0= Δc). One recognizes that A_T increases with σ^2_{lnk} and λ_y, but decreases with λ_x and Δc, i.e. $\{E(A_T) \sim \sigma_{lnk}^2, \lambda_y, 1/\lambda_x, 1/\Delta c\}$. This is in a good agreement with both the experimental results and the stochastic theory of Welty et al. (2003).

4. COMPARISON WITH ANALYTICAL STOCHASTIC THEORY

A theoretical formula proposed by Welty et al. (2003) for the transversal macrodispersivity in density-dependent flow could be developed further and now reads (Starke, 2005):

$$A_{33} = \frac{\sigma_f^2 \lambda_1 a_1}{\gamma_3^2}\{1 - a_2 \Gamma_3 \bar{x} G_3\} \qquad a_1 = \frac{\xi(2\xi+1)}{2(\xi+1)^2} \qquad a_2 = \frac{(\xi+1)^2}{2(1-\xi^2)(2\xi+1)} \tag{1}$$

where σ_{lnk}^2 is the variance of the log-normal permeability distribution; λ_1 and λ_3, the correlation lengths in directions x_1 and x_3; γ_3 the flow factor $\gamma_3 = v/(K_{ij}J_i)$; $\xi = \lambda_3 / \lambda_1$, an anisotropy factor; $\Gamma_3 = 2(dp/dx_3 - 0.65\rho_L g)/(dp/dx_3 - \rho_L g)\cdot\gamma_3^{-1}$, describing the density-dependence; G3, the concentration gradient dc/dx_3; and x, the mean displacement distance.

To validate this new formula above, the sets of experimental as well as numerical results obtained for $A_T = A_{33}$ are subject to a multiple linear regression analysis of the form $E(A_T) = X_1 b_1 + X_2 b_2$, whereby $X_1 b_1$ and $X_2 b_2$ denote density-independent and density- dependent

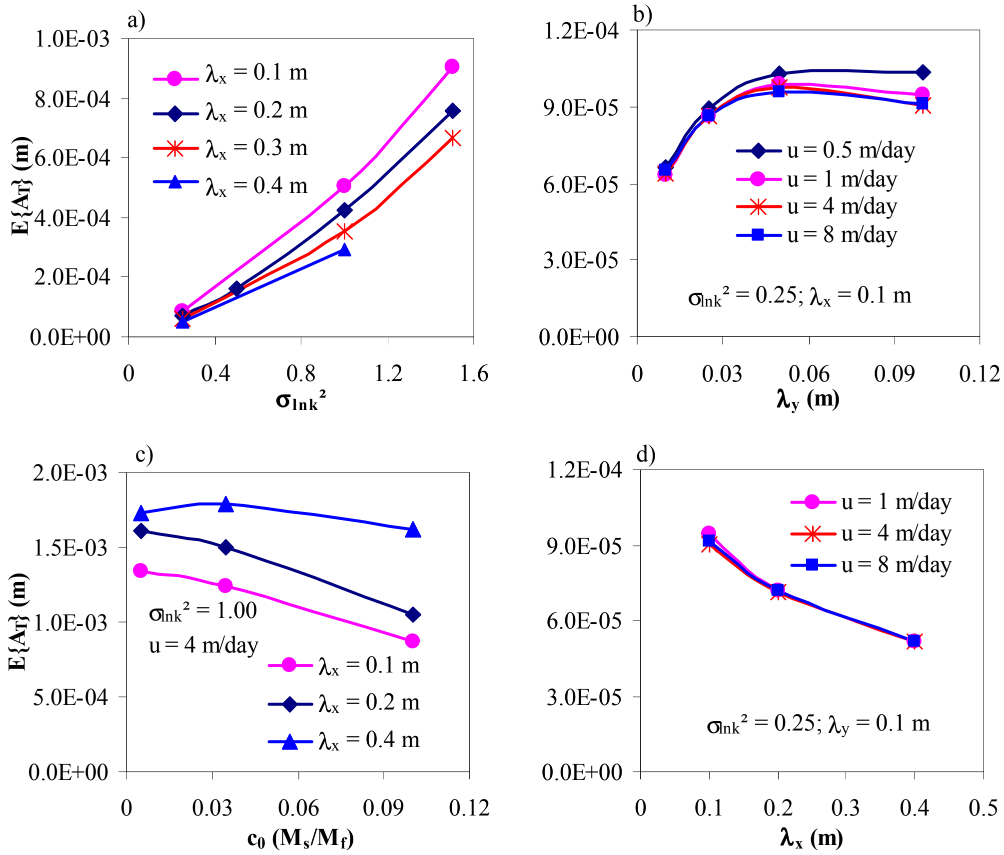

FIGURE 6: Monte Carlo simulated expectation values $E\{A_T\}$ as a function of various parameters of the porous medium (σ^2_{lnk}, λ_x, λ_y) and of the fluid (u, Δc).

factors, respectively, with $X_1$and X_2 comprising combinations of the known σ^2_{lnk}, λ_x , λ_y; and b_1, b_2 are unknown regressors of a combination of the flow factor γ and the density gradient dc/dx_3 and that are to be determined.

Carrying out the multiple regression analysis using formula (1) turned out to predict the values of A_T for both the tank experiments and the tracer (density-independent) MC-simulations very well (with an error probability $p<10^{-10}$) and, somewhat less satisfactory, for the density-dependent MC-runs ($p\sim0.05$) (cf. Starke, 2005, for details). We also observed that, for the tracer flow cases, the regression fits best when the flow factor γ is taken as constant, whereas for the density-dependent flow cases, γ is to be assumed a function of Δc of the flow and of the heterogeneity H of the medium.

5. SENSITIVITY ANALYSIS OF THE MACRODISPERSIVITY

To understand which characteristic parameter P_i of both the porous medium and the fluid flow affect the observed/computed macrodispersivities A_T the most, a sensitivity value S_i were computed through $S_i = P_i/A_T(P_i)*\partial A_T/ \partial P_i$, with P_i ε $\{\sigma_{lnk}^2,\lambda_x,\lambda_y ,p_{BC}, a_T, a_L, u, c_0\}$. It was recognized that the choice (cf. Koch and Starke, 2003) and the values of the pressure BC p_{BC} at the vertical boundaries of the tank have a large effect on A_T, as they influence strongly the vertical flow regime, leading to vertical displacements of the salt-freshwater interface (Fig. 7) and, also, to return flow from the outlet chamber back into the tank, effecting the concentration profiles in the rear sections of the former (cf. Koch and Starke, 2003, Starke, 2005, for details). The sensitivity of A_T to the local dispersivities a_L and a_T used in the transport model and to the concentration difference c_0 is not very strong and decreases with increasing heterogeneity $H \sim \sigma_{lnk}^2 * \lambda_x$ of the porous medium, with the latter having, through the value of σ_{lnk}^2, the largest impact on the transversal macrodispersivity measured.

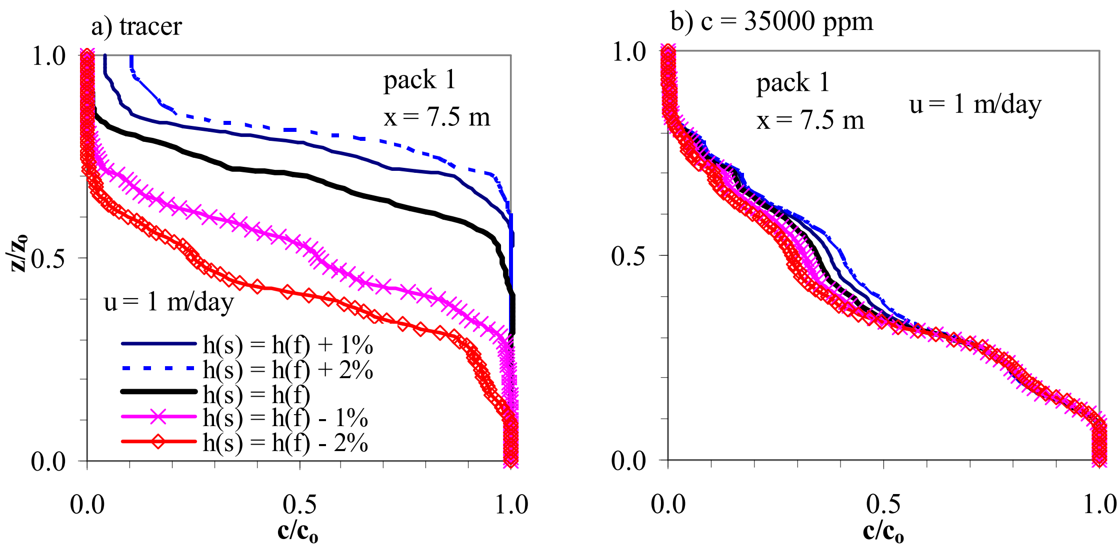

FIGURE 7. Effects of varying the head around a reference value on the vertical locations of the salt-freshwater interface for, a) tracer, b) density-dependent case.

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