On the use of random conductivity fields to promote unstable flow of dense plumes

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Abstract Flow under variable-density conditions is widespread, occurring in geothermal reservoirs, at waste disposal sites or due to saltwater intrusions. In nature, the migration of dense plumes typically results in the formation of vertical plume fingers which are known to be triggered by material heterogeneity. Random hydraulic conductivity (K) fields are introduced into numerical simulations to incorporate pore-scale heterogeneity into homogenous media and to generate fingers realistically. That method is evaluated using a previously-conducted laboratory-scale sand tank experiment, which is numerically re-simulated here. Results indicate that the variance of ln(K) of 10^{-3} (K in m s^{-1}) realistically reproduces the number of plume fingers observed in the sand tank experiment. Introducing random K fields is therefore useful to accurately simulate dense plume fingering in saturated homogeneous porous media. A Monte Carlo approach showed that the simulation of dense plume fingers is realisation-independent.

Key words model; groundwater; saturated; density; fingering; random K field; Monte Carlo

INTRODUCTION

Leachate that invades soil, e.g. from waste disposal sites, frequently possesses high solute concentrations and therefore higher fluid densities than ambient freshwater. In nature, the migration of dense plumes through a porous medium typically results in the formation of lobe-shaped instabilities or vertical plume fingers, which are known to have a non-negligible effect on the propagation of the plume. Flow direction in plume fingers is downwards, counterbalanced by upwards flow of less dense fluid between the fingers. In heterogeneous media, heterogeneity itself is known to trigger the formation of dense fingers. However, in homogeneous media fingers are also created even though all grains may have the same diameter. The reason can be assumed to be that pore-scale heterogeneity leading to different flow velocities also exists in homogeneous media due to two effects: (a) grains of identical size may randomly arrange differently, thus forming tetrahedrons, hexahedrons or octahedrons, where each arrangement creates pores of varying diameter, which results in different average flow velocities, and (b) random variations of solute concentration lead to varying buoyancy effects, thus also resulting in different pore-scale velocities. In numerical simulations, adequately incorporating those two effects remains a challenging task. One may suggest that numerical errors occurring during the computing process may perturb the flow field. However, the problem with this approach lies in the fact that numerical errors "may occur by themselves and are uncontrollable as location and magnitude of the error may vary with time. Small changes to dispersion parameters, time step sizes, or spatial discretization throughout a series of simulations can cause different instabilities to form" (Simmons *et al.*, 1999). Hence, deliberately triggering instabilities by small perturbations represents a controlled way to account for pore scale heterogeneity. Perturbations can be introduced through several variables, e.g. concentration of the solute or variance in K field, and numerous ranges, e.g. perturbation of solute source or whole area. Many publications exist where deliberate, artificially generated perturbations have been successfully utilised, e.g. Simmons *et al.* (1999) or Johannsen *et al.* (2006). However, detailed investigation and evaluation of the perturbation methods is rarely performed. Therefore, the objective of the present paper is to evaluate the use of random K fields to perturb flow, thereby incorporating pore-scale heterogeneity such that dense fingers are being realistically generated. Success of this perturbation method is validated by comparison of numerical results with a laboratory experiment (Simmons *et al.*, 2002).

PHYSICAL MODEL

Simmons *et al.* (2002) conducted laboratory experiments of variable-density flow and salt transport in a 2D vertical sand tank. Ambient horizontal flow was not simulated, and the groundwater table was constant. The focus was therefore put on variable-density free convective flow, including the generation of dense salt fingers. Stained calcium chloride solutions of variable density were introduced along the upper boundary. In the saturated high density (SHD) case, the introduced solution had a density of 1235 kg m^{-3}. The density difference between freshwater initially filling the entire tank and the dense calcium chloride solution lead to downwards density-driven migration of plume fingers through the tank. The range of density used for the solutions is representative for density ranges encountered in natural groundwater systems.

NUMERICAL MODEL

The numerical variable-density flow and solute transport model HydroGeoSphere (Therrien *et al.*, 2009) is used here to re-simulate the SHD laboratory experiment conducted by Simmons *et al.* (2002). Geometry of the numerical simulation domain is identical to that of the laboratory experiment, and extensions are l_x = 1.178 m, l_y = 0.053 m and l_z = 1.060 m. The domain is discretized by 500 × 500 uniform hexahedral elements of size Δx = 2.356 mm, Δy = 53 mm Δz = 2.12 mm. Left, right and bottom boundaries are assumed to be impermeable for flow. The model represents ponding due to injection of the solute source by a constant equivalent freshwater head boundary condition that is h_0 = 0.42 cm for the solute source and h_0 = 0 m on both sides of the source. All boundaries are zero-dispersive flux boundaries except the solute source where the constant relative concentration c = 1 (corresponding to C_{max} = 313 060 mg L^{-1}) is assumed. Initial conditions are h_0 = 0 m for flow, and c = 0 for transport. Total simulation time is 1 h, and time step size is assumed to be adaptive such that concentration does not vary by >0.01 during a single time step. Dimensions, initial and boundary conditions are shown in Fig. 1, and physical parameters are listed in Table 1.

RANDOM K FIELD

The laboratory experiment exhibits vivid fingering where the downwards movement of numerous small dense plume fingers is counterbalanced by upwards movement of freshwater. In a first numerical simulation using a homogeneous K field, that fingering pattern could not be reproduced, and four large fingers were being simulated (results not shown) instead of numerous small fingers

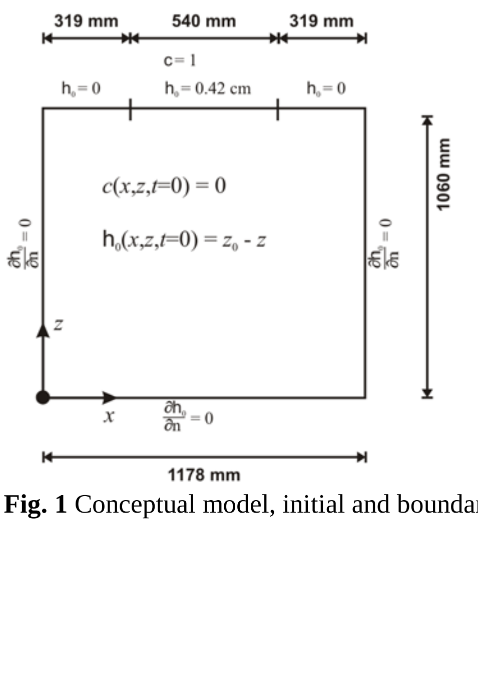

Fig. 1 Conceptual model, initial and boundary conditions.

Table 1 Material parameters used in numerical simulations.

Parameter	Value
Freshwater density (ρ_0)	1000 kg m^{-3}
Maximum fluid density (ρ_{max})	1235 kg m^{-3}
Maximum fluid concentration (C_{max})	313 060 mg L^{-1}
Porosity (Φ)	36 %
Hydraulic conductivity (K)	0.00163 m s^{-1}
Fluid dynamic viscosity (μ)	10^{-3} kg m^{-1}s^{-1}

as simulated physically. Therefore, in order to trigger fingering in the numerical solution, random hydraulic conductivity fields (random K fields) are being generated, and it is assumed that the random K variations represent pore-scale heterogeneity of the sand in the laboratory tank. The K fields are generated with a random K field generator using a stochastic Gaussian covariance model. By applying a variance to ln(K), a set of spatially variable K-values is generated where each value is associated to an element in the numerical grid, and where the K-values vary around the mean K-value of 0.00163 m s^{-1}. Variance is chosen such that it induces physically insignificant but numerically significant heterogeneity. Although the field generator offers the possibility to create correlated anisotropic random fields, solely random uncorrelated isotropic fields are used in the present study because the laboratory soil is isotropic and homogeneous on the laboratory (metre) scale. Therefore, a random white noise as shown in Fig. 2 is applied to perturb the variable-density flow field. To determine the appropriate variance of ln(K) that correctly reproduces the result of the SHD laboratory experiment, six K fields with different ln(K) variances reaching from 10^{-1} to 10^{-6} (K in m s^{-1}) are used to numerically re-simulate the SHD experiment. In a second step, the variance giving the best fit between laboratory and simulated fingers is used to generate a number of realisations in order to determine deviations in flow behaviour occurring solely due to randomness of the K field.

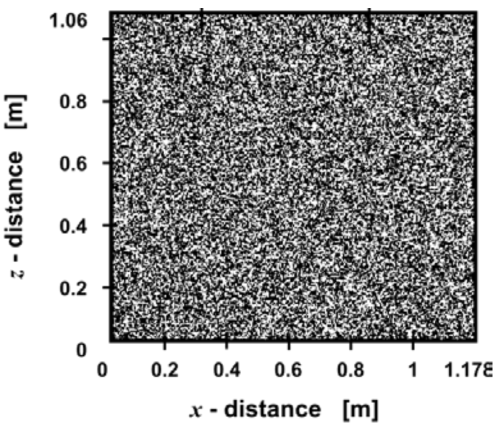

Fig. 2 Random conductivity (K) field.

RESULTS AND DISCUSSION

Figure 3 shows results of the SHD laboratory experiment, and its numerical simulation with a ln(K) variance of 10^{-3} after 20 minutes of plume transport. Clearly, number of dense fingers, size of fingers, downwards migration speed, and convective pattern are very similar. This observation indicates that using random K fields in the simulation of dense plume transport realistically reproduces plume fingering.

Figure 4(a) shows the number of fingers for the laboratory experiment as well as for the numerical simulations of six different variances (10^{-1} to 10^{-6}) of ln(K) *versus* time. Results indicate that variances of ln(K) that are equal to or smaller than 10^{-6} can be considered as homogeneous K fields because the number of fingers and the solute migration pattern are identical to the case mentioned earlier where K was assumed identical in the numerical simulation. Figure 4(b) shows the error between physically and numerically simulated number of salt fingers evaluated in the L2-Norm. Clearly, the error generally decreases as variance increases and a minimum is obtained for the variance 10^{-3}. Therefore, that variance is used here to simulate dense plume transport on a number of realisations of the K field.

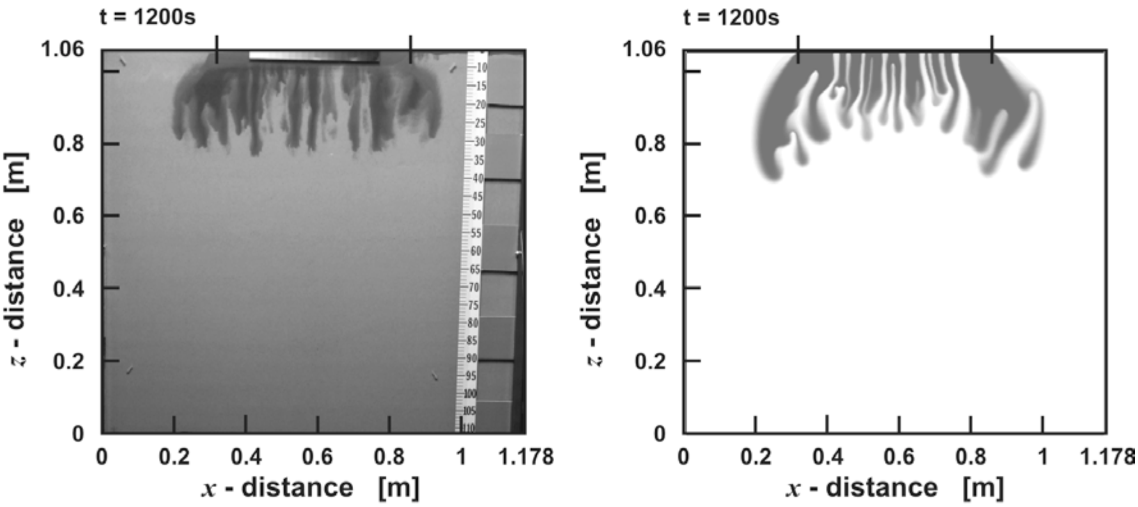

Fig. 3 Comparison of laboratory (left) and numerical (right) experiment where the variance of ln(K) is 10^{-3}.

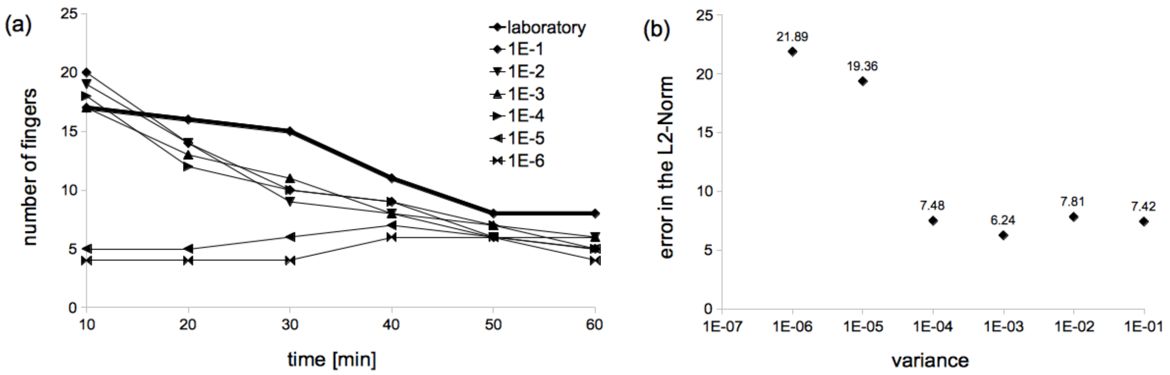

Fig. 4 (a) Number of fingers *vs* time for the laboratory experiment as well as for the six numerical simulations where different variances (10^{-1} …10^{-6}) of ln(K) are used, and (b) error between physically and numerically simulated number of plume fingers in the L2-Norm.

A Monte Carlo approach was used where eight realisations of the numerical SHD simulation with the ln(K) variance of 10^{-3} were carried out. To quantify differences between realisations and to verify convergence of the Monte Carlo approach, the averaged cumulative number of fingers is calculated and shown in Fig. 5(a). The error between the averaged cumulative number of fingers from all i and all i+1 realisations is evaluated in the L2-Norm and shown in Fig. 5(b). Figure 5 indicates that the average number obtained from all eight realisations is nearly identical to the results from only one realization. This indicates that a Monte Carlo approach is not required to realistically simulate dense plume fingering in homogeneous saturated porous media. Small differences that do exist between all i and all i+1 realisations clearly converge to zero, as demonstrated in Fig. 5(b).

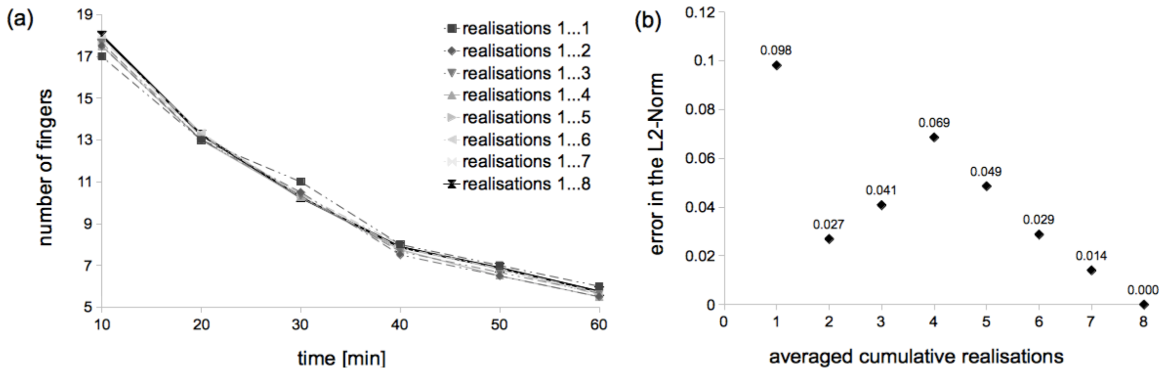

Fig. 5 (a) Averaged cumulative number of fingers, (b) Error between averaged cumulative number of fingers from all i and all i+1 realisations in the L2-Norm.

CONCLUSIONS

To the authors' knowledge, this is the first study that systematically investigates the effect of a random K field on the numerical generation of dense plume fingers in saturated homogeneous porous media. Results of this study indicate that:

(a) introducing a random K field is very useful to accurately reproduce dense plume fingering,

(b) the number of numerically simulated plume fingers corresponds to the physically simulated number of fingers if the variance of the ln(K) field is 10^{-3} (K in m s^{-1}), and

(c) a Monte Carlo approach is not required because an increased number of realisations did not significantly change the numerical result.

Upcoming studies will focus on other mechanisms to numerically perturb a variable-density flow field (e.g. random noise of solute source concentration, random noise of simulated concentration, etc.) to realistically simulate dense plume fingering.

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