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Density-dependent dispersion in heterogeneous porous media
Part I: A numerical study

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Abstract

In this paper, we describe carefully conducted numerical experiments, in which a dense salt solution vertically displaces fresh water in a stable manner. The two-dimensional porous media are weakly heterogeneous at a small scale. The purpose of these simulations, conducted for a range of density differences, is to obtain accurate concentration profiles that can be used to validate nonlinear models for high-concentration-gradient dispersion. In this part we focus on convergence of the computations, in numerical and statistical sense, to ensure that the uncertainty in the results is small enough.

Concentration variances are computed, which give estimates of the uncertainty in local concentration values. These local variations decrease with increasing density contrast. For tracer transport, obtained longitudinal dispersivities are in accordance with analytical findings. In the case of high-density contrasts, stabilizing gravity forces counteract the growth of dispersive fingers, decreasing the effective width of the transition zone. For small log-permeability variances, the decrease of the apparent dispersivity that is found is in agreement with laboratory results for homogeneous columns.

Keywords: Heterogeneous porous media; High-concentration-gradient dispersion; Brine transport; Solute transport; Density-dependent flow; Macrodispersion; Stochastic media; Concentration variance

1. Introduction

1.1. High-concentration-gradient dispersion

This numerical study is part of an investigation of the nonlinear effects that occur when dispersive transport is affected by large density differences. From laboratory experiments it has become clear that the commonly used linear Fickian-type law for dispersion no longer holds when concentration gradients become large. As a result of density gradients, gravity plays a stabilizing or destabilizing role depending on the configuration. In the stable case this results in a reduction of dispersive mixing and smaller effective dispersivities. For a short overview of this topic we refer to Schotting and Landman [35].

The laboratory experiments that were performed on high-concentration-gradient dispersion by Bouhroum [7], Hassanizadeh et al. [19], Moser [32], and Anderson [1] were essentially one-dimensional. In this study, we consider the same simple configuration, with unidirectional mean flow. However, on the small scale of heterogeneities the flow is two-dimensional. This is the scale where the interaction between density gradients and gravity is affecting the dispersive spreading. These processes are mimicked in detail in a two-dimensional (2D) heterogeneous porous medium. Next, the computed concentrations are averaged over the

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horizontal (transversal flow) direction. The obtained upscaled behavior can be described by a one-dimensional (1D) model and compared to the various laboratory experiments [1,7,19,23,28,32]. The study is limited to stable displacements: fresh water is always on top of the heavier salt water solution. Our purpose is to obtain numerical results that can be used to validate newly developed models for nonlinear high-concentration-gradient dispersion, among which the one proposed by Hassanizadeh and Leijnse [18]. In this paper, we focus on convergence in a numerical and statistical sense, and estimate the uncertainty in the results. Moreover, a comparison with laboratory experiments is made.

1.2. Stochastic transport

In this section, some observations with regard to transport in stochastic media are reviewed that are relevant to this study. Dispersion of non-reactive tracers has been the subject of many studies. It is common to describe the heterogeneous porous medium in terms of stochastic parameters. Generally, the permeability is assumed to be log-normally distributed, characterized by a mean value and a variance. The correlation function describes how permeability values are spatially correlated, where the correlation scale can be interpreted as a measure of the characteristic size of heterogeneities. However, even in cases where the domain under consideration is large compared to the correlation scale, the uncertainty in predicted concentration values can be very large. Individual porous media replica's with the same statistical characteristics can generate very different results. Therefore, averaging over an ensemble of realizations is necessary in order to obtain statistically meaningful results.

In the famous work of Gelhar and Axness [16], expressions for macroscale dispersion coefficients are given in terms of the stochastic parameters for both isotropic and anisotropic porous media. Their analysis is valid in the limit of large displacements only, when the scale of the flow system is large compared to the correlation scale. Dagan's theory [10] is able to describe the evolution of macrodispersivity with time, and for large time approaches the results of Gelhar and Axness. From numerous numerical and theoretical studies on dispersive tracer transport in stochastic media, some conclusions can be drawn that are of interest for this study:

(1) Under ergodic conditions, dispersion coefficients tend to constant values after tens of correlation lengths (Dagan [10]). The ergodic hypothesis holds for averaging over large areas compared to the correlation scale, or equivalently over an ensemble of realizations.
(2) For single realizations there is no evidence that asymptotic macrodispersivities are reached, even after hundreds of correlation lengths (Trefry et al. [38]). According to Dagan [11], ergodic conditions are eventually reached in the limit $t \to \infty$, but for small initial solute source sizes compared to the correlation scale, travel times need to be extremely large to reach the asymptotic limit.
(3) Results differ greatly between individual porous medium realizations having the same stochastic parameters (Smith and Schwartz [37]). Therefore, to make predictions of solute concentrations in field situations (single realizations), not only ensemble averaged results are needed but also a measure of the deviation (uncertainty).
(4) The uncertainty in concentration values in single realizations can be very large, and is highest in areas where the concentration gradients are large (Graham and McLaughlin [17], Vomvoris and Gelhar [40], Cvetkovic et al. [9]). The uncertainty decreases with increasing microscale (pore scale) dispersion (Black and Freyberg [6], Graham and McLaughlin [17], Kapoor and Gelhar [27], Dagan and Fiori [12], Andričević [2]).
(5) Where breakthrough is considered at a plane transversal to the flow direction, the uncertainty in the averaged concentration decreases with increasing size of the averaging area (3D) or line (2D) (Black and Freyberg [6], Cvetkovic et al. [9], Dagan and Fiori [12]).

Applying the above to the problem under consideration here, it is not to be expected that single realization results yield constant dispersion coefficients after 10s or even 100s of correlation lengths. Averaging needs to be done over a number of realizations, depending on the width of the column with respect to the correlation length. In order to make predictions for field situations, it is important to know how strongly concentrations in individual realizations (or in the field) may deviate from their ensemble average. Therefore, we investigate the topic of concentration variance thoroughly. The relevance of this topic has been emphasized by various authors, e.g. Smith and Schwartz [37], Vomvoris and Gelhar [40], and Kapoor and Gelhar [26]. New in the present study is the effect of (stabilizing) density gradients on the concentration variance.

1.3. Outline

The outline of this paper is as follows. In Section 2 the numerical model and its assumptions are presented. Section 3 discusses the numerical convergence and accuracy of the computations, as well as the convergence in a statistical sense. The influence of the density contrast on both types of convergence is discussed. Estimates of the errors caused by the numerical scheme and by the use of a finite number of realizations are given and compared. In Section 4 results are presented and the differences between tracer and high-density transport are analyzed, for their concentration profiles, concentration variances, and macrodispersivities. For tracer transport, longitudinal macro-