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ScienceDirect
Advances in Water Resources 29 (2006) 1690–1704
Advances in Water Resources
www.elsevier.com/locate/advwatres

Numerical simulation of three-dimensional saltwater–freshwater fingering instabilities observed in a porous medium

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Received 1 December 2004; received in revised form 18 December 2005; accepted 18 December 2005
Available online 7 February 2006

Abstract

We consider saltwater–freshwater fingering instabilities in a saturated porous medium. In the first part, we present three-dimensional results obtained from a laboratory experiment using non-invasive imaging. In the second part, we define a set of model problems in which the performed laboratory experiments can be ranged in. Due to its highly non-linear behavior and inevitable modeling errors, a detailed numerical reproduction of the physical concentration measurements cannot be expected. Nevertheless, four criteria have been identified, two quantitative and two qualitative, which facilitate a substantiated comparison of the physical experiment and the numerical simulation. With respect to these criteria a high degree of similarity could be observed. The use of these features allows a deeper understanding of the physical processes and the influence of the initial conditions.

Keywords: Porous media; Variable-density flow; Saltwater; Instability; Multigrid methods; Non-invasive imaging; NMR

1. Introduction

In groundwater environments, fluid density and viscosity are generally variables related to the concentration of solutes, temperature, or pressure conditions. Both fluid properties may alter the flow patterns and prevailing flow regimes. For variable density flow conditions, this becomes evident in a number of field situations. Among those are convective flows in geothermal systems, flows around salt domes, leaching and disposal of dense solutes or brines, or saltwater fingering below playa lakes and salt pans. These situations have been subject to long-standing investigation and numerical analysis. The variety of findings and current challenges are stated in, e.g. [45,46], whereas a recent review of the literature on the numerical treatment is given in [11]. We refer to these reviews for details and references.

Due to the non-linear coupling of the equations for density-dependent flow and solute transport, their solution is more complex than for the case of passive tracer transport. Density-dependent flows are rotational and hydrodynamic instability leading to a non-uniqueness of the solution is inherent in the mathematical and physical models of such systems. The criterion for instability that is investigated theoretically, experimentally and numerically is typically expressed in form of a Rayleigh number *Ra*. This dimensionless ratio of buoyancy to diffusion and dispersion is derived under a steady-state flow assumption.

The experimental investigation of gravitationally unstable flow configurations, i.e. light fluid underlying a heavier fluid, mainly employed pseudo-two-dimensional Hele-Shaw setups to study the thermal instability in Rayleigh–Bénard convection [13,43,54], the Rayleigh–Taylor

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0309-1708/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.advwatres.2005.12.008

instability in porous media [14,40] or instability induced below an evaporation boundary [55,56]. The number of experiments in real porous media in three-dimensional setups (as opposed to Hele-Shaw cells) is very limited to date [6,29,31,42]. This paper presents a fully three-dimensional dataset of solute concentrations during the process of purely density-driven miscible fingering in a benchmark scale setup. The experiment was designed especially for subsequent numerical simulation, providing all required parameters.

High-accuracy, three-dimensional numerical studies were carried out to investigate the mechanisms affecting hydrodynamic instabilities in miscible displacement for well-defined geometries, e.g. resolving the gap of Hele-Shaw cells [14,27], for rectilinear geometries [49,57] or for quarter five-spot configurations [38]. Difficulties in the numerical handling were found to be closely connected to the geometries of the domain, the spatial variability of the base flow and the presence of line sources and sinks, cf. [28]. The numerical issues concerned the inaccurate representation of velocity variations and grid-orientation effects that superimpose numerical artifacts on the model predictions. This can even lead to unphysical numerical results, particularly in highly non-linear systems. We provide a numerical simulation approach that is able to reproduce the physical experiment with sufficient numerical accuracy. Notably, such detailed simulations of miscible fingering are to date rare in three dimensions.

The early analytical work [9,21,40] treated instability of miscible fluid displacement in porous media with a first-order perturbation approach. The motion of two incompressible fluids separated by a sharp interface in a porous medium was based on Hele-Shaw equations, or Darcy's law. The high sensitivity of the problem to perturbations is caused by singularity in the governing equations in the absence of surface tensions or dispersive mechanisms. In miscible displacements in realistic porous media, flow-induced dispersion plays a dominant role by widening the front and thereby yielding a cut-off length scale for the potential growth of instabilities [36]. The cross-over between diffusive and linear growth regimes was analyzed by, e.g. [48,53]. Subsequently, Coskuner and Bensten [10] or Bacri et al. [2] proposed an extended theory for the prediction of a stability criterion for miscible displacement in porous media taking a velocity-dependent dispersion tensor into consideration. In a recent treatment, the linear stability analysis was performed on the basis of the three-dimensional Stokes equations [16], thus accounting for Taylor dispersion at the interface due to gradients in the velocity field. This enabled the prediction of a wavelength selection for Hele-Shaw configurations across high *Ra* and low *Ra* regimes.

Linear stability analysis of dominant modes that evolve from interface perturbations considers the exponential growth regime of the characteristic initial wavelengths. Such analysis applies strictly to the short time scales. A weakly non-linear analysis of the formation of finger patterns was very recently presented by Alvarez-Lacalle et al. [1] and Casademunt [8] for dynamical system conditions. A formal gradient expansion of the non-local problem allowed the exact determination of a subcritical bifurcation for the Saffman–Taylor instability. Such dynamic analytical analysis is beyond the scope of this contribution. Our setup also included a marked heterogeneity in the porous medium, a situation which has not been fully incorporated in stability analyses. Here, we analyze a reproducible setting of dynamically evolving finger instabilities by comparing computations in analogy to a three-dimensional, physical pattern evolution.

Previously, we presented comparisons between an experimental investigation and numerical simulation for stable density-dependent flow configurations, or upconing conditions [25,33]. The study provided a mathematical benchmark for numerical modeling of density-dependent flow, in a three-dimensional setting and for the case of strong density coupling. The non-linearity in the density unstable model system can be significantly higher, and poses in itself numerical challenges. Benchmarking issues for unstable convection in two-dimensional configurations have been addressed more recently by Weatherill [52] under steady-state conditions in finite and infinite, bound horizontal or inclined layers, or by Simmons et al. [47] for transient conditions for the two-dimensional salt lake problem with an unstable saline boundary layer formed by evaporation. In the latter test case, the hydrodynamic instability proved to be far more sensitive to the initial perturbations than for the purely diffusive regime studied in [52]. The conditions pertaining in field problems necessitate the further development and testing of numerical tools for three-dimensional, transient instabilities. In this contribution we examine saltwater–freshwater fingering in three dimensions in a porous medium. We present, for the first time to our knowledge, a fully three-dimensional, high-quality dataset of solute concentrations during the process of purely density driven miscible fingering in a porous medium for a bench scale setup. Moreover, this also comprises the effects of a permeability heterogeneity and was designed especially for subsequent numerical simulation, thus delivering all the required parameters. We provide a numerical simulation approach that is able to represent the situation and processes of the physical experiment with a reasonable numerical accuracy. Notably, such detailed simulations of miscible fingering are quite common in 2D, but are so far very rare in 3D. We develop a framework for comparing experimental and numerical results in a meaningful way. This is not trivial for such a highly non-linear behavior, which strongly amplifies perturbations, and cannot be performed as a direct comparison on a point-to-point basis as is typical for other situations. Finally, we demonstrate the capability of the numerical model to capture the essential behavior of the physical process to a high degree, and then to look at the influence of initial conditions, which could not be done so easily in a physical experiment.