Journal of Hydrology 542 (2016) 541–551

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Research papers

Representativeness of 2D models to simulate 3D unstable variable density flow in porous media

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A R T I C L E   I N F O

Article history:
Received 1 March 2016
Received in revised form 29 August 2016
Accepted 9 September 2016
Available online 14 September 2016
This manuscript was handled by P. Kitanidis, Editor-in-Chief, with the assistance of Jian Luo, Associate Editor

Keywords:
Variable density flow
Porous media
Column experiments
Numerical modelling

A B S T R A C T

Variable density flow in porous media has been studied primarily using numerical models because it is a semi-chaotic and transient process. Most of these studies have been 2D, owing to the computational restrictions on 3D simulations, and the ability to observe variable density flow in 2D experimentation. However, it is recognised that variable density flow is a three-dimensional process. A 3D system may cause weaker variable density flow than a 2D system due to stronger dispersion, but may also result in bigger fingers and hence stronger variable density flow because of more space for fingers to coalesce. This study aimed to determine the representativeness of 2D modelling to simulate 3D variable density flow. 3D homogeneous sand column experiments were conducted at three different water flow velocities with three different bromide tracer solutions mixed with methanol resulting in different density ratios. Both 2D axisymmetric and 3D numerical simulations were performed to reproduce experimental data. Experimental results showed that the magnitude of variable density flow increases with decreasing flow rates and decreasing density ratios. The shapes of the observed breakthrough curves differed significantly from those produced by 2D axisymmetric and 3D simulations. Compared to 2D simulations, the onset of instabilities was delayed but the growth was more pronounced in 3D simulations. Despite this difference, both 2D axisymmetric and 3D models successfully simulated mass recovery with high efficiency (between 77% and 99%). This study indicates that 2D simulations are sufficient to understand integrated features of variable density flow in homogeneous sand column experiments.

1. Introduction

Density driven flow is an essential process for describing solute transport in porous and fractured systems where fluid flow is driven by a variation in density. Variations in density can be caused by solute concentration, temperature and/or pressure of a fluid (Simmons, 2005; Simmons et al., 2001). In particular, this density driven flow is of strong relevance to practical issues including salt water intrusion (Huyakorn et al., 1987; Pinder and Cooper, 1970; Van Dam et al., 2009; Voss and Souza, 1987), contaminant transport (Frind, 1982; Oostrom et al., 1992a, 1992b; Schincariol and Schwartz, 1990), contamination site remediation (Flowers and Hunt, 2007) and nuclear waste disposal (Hassanizadeh and Leijnse, 1988; Herbert et al., 1988). Depending on several factors (i.e., porous medium permeability, porosity, water flow velocity and density ratio of intruding fluid to ambient groundwater), density driven flow can become unstable under certain circumstances (Biggar and Nielsen, 1964; Krupp and Elrick, 1969; Rose and Passioura, 1971). Unstable density driven flow is characterised by the formation of finger-shaped instabilities with density constantly varying in space and time. This unstable density driven flow (or variable density flow) is superimposed onto regional groundwater flow and hence can cause more widespread aquifer contamination by distributing contaminants vertically (Beinhorn et al., 2005; Flowers and Hunt, 2007). Being able to reliably understand, observe, measure, simulate and predict variable density flow is a critical challenge for hydrogeology (Simmons, 2005).

Variable density flow has been studied primarily through 2D settings to investigate onset, growth and decay of instabilities (e.g., Voss and Souza, 1987; Xie et al., 2010, 2011, 2012; Riaz et al., 2006; Jang and Aral, 2007; Prasad and Simmons, 2003, 2005). The implicit assumption of 2D studies is that mixing is not important in the direction orthogonal to the 2D planes and that a 2D transect is representative of a 3D system. Although this assumption is not valid in the real world, most studies have

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http://dx.doi.org/10.1016/j.jhydrol.2016.09.026
0022-1694/

nevertheless adopted it for simplicity. There has been little attempt to test, justify and discuss the assumptions made with respect to dimensionality and the effects it may have on flow and transport behaviour and model results. For example, Xie et al. (2010) modified the classic 2D Elder problem to examine the effect of time-varying salt loading on variable density flow. Riaz et al. (2006) performed 2D numerical modelling to verify predictions about instability onset time made by linear stability analysis in the context of carbon dioxide sequestration within saline aquifers. Van Dam et al. (2009) established several 2D transects to capture salty fingers using geophysical methods. Simmons et al. (2002) and Post and Simmons (2010) used the same 2D sand tank to investigate the fingering process in a variable saturated setting and a heterogeneous setting, respectively. Those lab and field studies have also been reproduced in 2D numerical models (Cremer and Graf, 2015; Dam et al., 2014; Post and Simmons, 2010). However, as shown by these 2D numerical studies, precise reproduction of field and experimental observations is hard due to the transient and semi-chaotic nature of variable density flow. van Reeuwijk et al. (2009) demonstrated that the classic Elder problem – a typical variable density flow system – is characterised by multiple steady state solutions. Despite this inherent issue in variable density flow, prior 2D numerical modelling studies have also indicated that reliable predictions of variable density flow can still be made if we use macroscopic features such as integrated solute mass flux, total solute mass and centre of gravity (Prasad and Simmons, 2003, 2005; Xie et al., 2012). These studies still remain 2D studies, with 2D representations of 3D realities.

3D studies are challenging and hence rare because they create increased computational burden in a numerical study and fingering patterns are challenging to visualise in an experimental setting. However, it is well recognised that variable density flow occurs in three dimensions (Diersch and Kolditz, 1998; Johannsen et al., 2006; Oswald et al., 1997; Pau et al., 2010). Both Oswald et al. (1997) and Johannsen et al. (2006) have attempted to reproduce experimental results with 3D numerical simulations. Oswald et al. (1997) found that the growth speed was reproduced correctly but the onset of instabilities was delayed in the 3D simulations. Johannsen et al. (2006) found that a detailed reproduction of observed fingering processes in the Salt Pool Problem (Oswald and Kinzelbach, 2004) cannot be obtained in the 3D simulations due to uncertainties in initial conditions and numerical errors. In addition, Diersch and Kolditz (1998) and Pau et al. (2010) simulated variable density flow in different settings only using 2D and 3D numerical models. Diersch and Kolditz (1998) extended the 2D Elder Problem to 3D. They observed similar upwelling salinity patterns in the centre of the model domain in both 2D and 3D scenarios. In the simulations of CO_2 sequestration, Pau et al. (2010) reported that the onset time of instabilities was shorter and the magnitude of the stabilized CO_2 flux was higher in 3D than in 2D. However, they argued that these differences are moderate in comparison to heterogeneities which can be normally found in geological media.

Although 3D studies do appear to become a little more common, there has not been a systematic comparison between lab or field observations, 2D and 3D numerical simulations on variable density flow. In comparison to 2D, a 3D system allows solute to migrate freely in all directions. On one hand, this freedom may result in stronger dispersion and possibly weaker variable density flow. On the other hand, it is also likely that fingers may grow bigger and so penetrate faster under gravitational influence in a 3D system. Whether 3D behaviour and modelling promotes or suppresses fingering process in mixed convective systems compared to 2D counterparts has not been examined yet.

In this study, we attempted to replicate observations in 3D lab experiments using both 2D axisymmetric and 3D numerical models. The objectives were to semi-quantitatively compare processes in 2D axisymmetric and 3D settings and also thoroughly examine the ability of 2D axisymmetric models to represent physical processes in 3D. We based this comparison on tracer experiments conducted in saturated homogeneous sand columns at three different water flow velocities and three different density ratios.

2. Material and methods

In this study a Darcy column with a diameter of 4.8 cm and a length of 50.8 cm was used to perform experiments (Fig. 1). The porous medium in the column was comprised of coarse quartz sand (Dorsilit Nr. 5F, Quarzsande GmbH, Germany) with a particle size distribution between 1.0 mm and 1.8 mm, a porosity of n = 0.44 and a hydraulic conductivity of $k = 7.0 \cdot 10^{-3}$ m s^{-1} (605 m d^{-1}) determined with the constant head method (Klute and Dirksen, 1986). A thin layer of silicon adhesive was implemented between the column and the coarse sand to eliminate potential preferential flow paths along the column wall. The column was packed with the coarse sand under saturated conditions to avoid entrapped air bubbles. All experiments were run with deionized and filtered water (MilliQ, MilliporeElix + Milli-Q Advantage 10A, USA) constantly flowing from the bottom to the top using a peristaltic pump (Gilson Abimed Minipuls 3). A radial-distribution device was used to inject the inflow water evenly over the whole cross section of the column. The accuracy of the peristaltic pump was ±0.2 mL h^{-1}.

Bromide is known to be free of sorption (Levy and Chambers, 1987; Maloszewski et al., 1999) and was therefore used as a conservative tracer. Potassium bromide was dissolved in the deionized and filtered water to create a bromide solution with a concentration of 95 mg L^{-1}. This very low concentration did not significantly change the fluid density and so the fresh water density could be

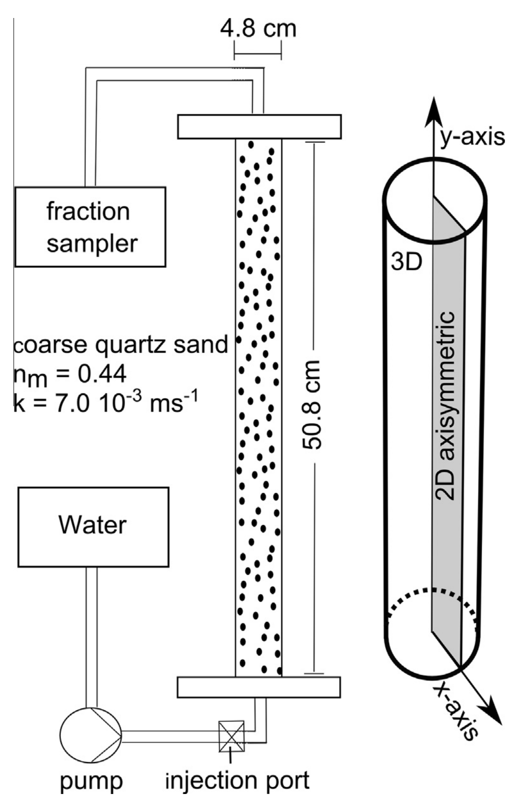

Fig. 1. Experimental design of the homogenous sand column and numerical model setup in 3D and 2D axisymmetric projection.