Journal of Contaminant Hydrology 173 (2015) 69–82

Contents lists available at ScienceDirect

Journal of Contaminant Hydrology

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

Generation of dense plume fingers in saturated–unsaturated homogeneous porous media

Clemens J.M. Cremer *, Thomas Graf

Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, Leibniz Universität Hannover, Appelstr. 9A, 30167 Hannover, Germany

ARTICLE INFO

Article history:
Received 7 July 2014
Received in revised form 10 November 2014
Accepted 26 November 2014
Available online 9 December 2014

Keywords:
Model
Groundwater
Saturated
Unsaturated
Density
Numerical trigger
Fingering

ABSTRACT

Flow under variable-density conditions is widespread, occurring in geothermal reservoirs, at waste disposal sites or due to saltwater intrusion. The migration of dense plumes typically results in the formation of vertical plume fingers which are known to be triggered by material heterogeneity or by variations in source concentration that causes the density variation. Using a numerical groundwater model, six perturbation methods are tested under saturated and unsaturated flow conditions to mimic heterogeneity and concentration variations on the pore scale in order to realistically generate dense fingers. A laboratory-scale sand tank experiment is numerically simulated, and the perturbation methods are evaluated by comparing plume fingers obtained from the laboratory experiment with numerically simulated fingers. Dense plume fingering for saturated flow can best be reproduced with a spatially random, time-constant perturbation of the solute source. For unsaturated flow, a spatially and temporally random noise of solute concentration or a random conductivity field adequately simulate plume fingering.

1. Introduction

Leachate that invades soil, e.g. from waste disposal sites, frequently possesses higher solute concentration and therefore higher fluid density than ambient freshwater.

Spatial variation of water density can lead to variable-density flow, which is a key process in the transport of contaminants, salt transport in coastal aquifers or hot geothermal plumes (Diersch and Kolditz, 2002; Illangasekare et al., 2006; Simmons, 2005; Simmons et al., 2001; Stöckl and Houben, 2012; Van Dam et al., 2009).

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 (Xie et al., 2011). Flow direction in solute plume fingers is downwards, counterbalanced by an upward flow of less dense fluid between the fingers. The generation of plume fingers can be attributed to material heterogeneity, which is known to trigger the formation of dense fingers (Goswami et al., 2011; Schincariol, 1998; Schincariol and Schwartz, 1990; Schincariol et al., 1997). In homogeneous media, however, fingers are also created even though the material is uniform with identical sizes of material grains (e.g. sand grains) (Goswami et al., 2011; Simmons et al., 2002; Van Dam et al., 2009; Wooding et al., 1997b). 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: (i) random variations of solute concentration leading to varying buoyancy effects, which results in different average flow velocities, and (ii) grains of identical size which may randomly arrange differently, thus forming tetrahedrons, hexahedrons or octahedrons, where each arrangement creates pores of varying diameters, thus also resulting in different pore-scale velocities.

Usually, variable-density flow models do not consider effects (i) and (ii), such that the numerical model does not apply any external perturbation to trigger plume fingering. In that case, numerical errors of the computing process are expected to

---

* Corresponding author.
E-mail address: cremer@hydromech.uni-hannover.de (C. Cremer).
URL: http://www.hydromech.uni-hannover.de (C. Cremer).

http://dx.doi.org/10.1016/j.jconhyd.2014.11.008
0169-7722/

perturb the flow field and to create unstable plume fingers. The problem with this approach, however, is that "these instabilities are not physically realistic and are essentially uncontrollable because their character depends on the extent to which numerical errors develop" (Schincariol et al., 1994). This has later been confirmed by Simmons et al. (1999) who noted 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." Xie et al. (2011) added that numerical errors are not easy to quantify.

As an alternative to relying on internal numerical errors, deliberately triggering instabilities by external perturbations represents a controlled way to account for pore-scale heterogeneity. Perturbations can be introduced through a noise applied to the solute concentration or through a random conductivity field.

List (1965) induced perturbations of the source concentration created by superposition of spatially oscillatory terms with sinusoidal form and performed a theoretical analysis on the relationship between the nature of the perturbation and the resulting instabilities. List (1965) identified the following parameters responsible for instability growth: the transverse Rayleigh number, the ratio of the transverse to the longitudinal Rayleigh numbers, and the nondimensional wave number. However, while List's stability theory provides a useful model for determining stability in a variable-density system, Schincariol (1998) criticized that the theory cannot account for dispersive dissipation of the dense plume as a function of travel distance and is therefore less useful in predicting the growth rate of instabilities in real systems.

Schincariol and Schwartz (1990) conducted physical experiments on the laboratory-scale in homogeneous, layered, and lenticular porous media in order to further investigate the influence of hydraulic conductivity and density differences on the formation of instabilities. It was observed that small density differences around 0.8 mg cm^{-3} between a higher density water overlying a less dense water results in the formation of gravitational instabilities. Schincariol et al. (1994) numerically reproduced the physical experiment by Schincariol and Schwartz (1990). Numerically generated errors and their influence on the development of instabilities were examined using the Courant- and Peclet-stability criteria. Schincariol et al. (1994) concluded that the formation of unstable flow depends on the Rayleigh-number and on the wavelength of the perturbation. Schincariol et al. (1997) and Schincariol (1998) tested the applicability of the stability theory developed by List (1965) to variable-density flow in homogeneous and heterogeneous media. Numerical simulations were carried out, where perturbations were induced by lab-scale heterogeneity of the conductivity field. Schincariol et al. (1997) concluded that besides the Raleigh number and wavelength, statistical characteristics of the conductivity field (mean, variance, correlation length scales) play an important role in the development of instabilities.

Simmons et al. (1999) numerically resimulated an experiment of an evaporating salt lake developed by Wooding et al. (1997a,b). A spatially and temporally random noise of the salt concentration in the lake was used to apply perturbation and to mimic field-scale heterogeneity. Using that perturbation technique, Simmons et al. (1999) could realistically reproduce experimental results by Wooding et al. (1997a,b). Xie et al. (2011) adopted this perturbation mechanism to study the effects of dynamic solute boundary conditions on the migration of dense plumes using the modified solute Elder problem (Voss and Souza, 1987). That problem was later reused and slightly modified in multiple realizations to analyze the speed of free convective fingering (Xie et al., 2012).

Weatherill et al. (2004) investigated the onset of convective roll instabilities due to thermal convection in a fluid-saturated porous layer that is uniformly being heated from below. The Horton–Rogers–Lapwood (HRL) problem (Horton and Rogers, 1945; Lapwood, 1948) was numerically resimulated with an initial perturbation at the domain center to initiate convection. A detailed investigation of that perturbation method is absent, and it therefore remains unknown whether the trigger used by Weatherill et al. (2004) really affects the onset of convection.

Recently, Illangasekare et al. (2006) and Van Dam et al. (2009) obtained evidence of lobe-shaped instabilities from field measurements. This highlights the importance of unstable density-driven flow in natural field settings and furthermore the importance of an adequate representation of these phenomena in numerical models.

The objective of the present study is to evaluate six different perturbation mechanisms in order to incorporate pore-scale heterogeneity into a numerical model such that dense fingers are realistically being generated under saturated and unsaturated flow conditions.

While partly relying on the evaluation of well known perturbation mechanisms, this study also introduces several mechanisms that are new to variable-density flow simulations. To the authors' knowledge, (i) a spatially and temporally random noise of solute concentration, (ii) the application of a spatially random, time-constant perturbation of the solute source, and (iii) a random conductivity field have previously not been examined as perturbation mechanisms in the literature of variable-density flow. Success of all perturbation methods is validated by comparison of numerical results with a physical laboratory model conducted by (Simmons et al., 2002).

2. 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 considered. The focus was put on variable-density free convective flow including the generation of dense salt fingers. Stained calcium chloride solutions of different densities were injected along the central part of the upper boundary. The experiments were carried out under fully saturated as well as partly saturated conditions. For the saturated case, injection of dense solutes created ponding along the source, such that the water table in the source was a few millimeters higher than those along the left and right top boundaries. The unsaturated experiment was carried out by draining the water level to 44 cm below the top surface of the sand. The present study focuses on the saturated high density (SHD) case and the unsaturated high density (UHD) case (Simmons et al., 2002) where the density of the source concentration was 1235 kg m^{-3}.

Fig. 1A and B presents the plume development of the physical SHD and UHD experiments after 40 min of dense