Journal of Contaminant Hydrology 138–139 (2012) 123–140

Contents lists available at SciVerse ScienceDirect

Journal of Contaminant Hydrology

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

Effects of domain shapes on the morphological evolution of nonaqueous-phase-liquid dissolution fronts in fluid-saturated porous media

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ARTICLE INFO

Article history:
Received 8 September 2011
Received in revised form 2 July 2012
Accepted 5 July 2012
Available online 14 July 2012

Keywords:
Nonaqueous phase liquid
Morphological evolution
Computational simulation
Domain shapes
Dissolution instability
Porous media

ABSTRACT

The main purpose of this paper is to investigate the effects of different domain shapes in general and trapezoidal domain shape in particular on the morphological evolution of nonaqueous phase liquid (NAPL) dissolution fronts in two-dimensional fluid-saturated porous media. After the governing equations of NAPL dissolution problems are briefly described, the numerical procedure consisting of a combination of the finite element and finite difference methods is used to solve these equations. The related numerical simulation results have demonstrated that: (1) domain shapes have a significant effect on both the propagating speed and the morphological evolution pattern of a NAPL dissolution front in the fluid-saturated porous medium; (2) an increase in the divergent angle of a trapezoidal domain can lead to a decrease in the propagating speed of the NAPL dissolution front; (3) the morphological evolution pattern of the NAPL dissolution front in a rectangular domain is remarkably different from that in a trapezoidal domain of a large divergent angle; (4) for a rectangular domain, the simplified dispersion model, which is commonly used in the theoretical analysis and numerical simulation, is valid for solving NAPL dissolution instability problems in fluid-saturated porous media; and (5) compared with diverging flow (when the trapezoidal domain is inclined outward), converging flow (when the trapezoidal domain is inclined inward) can enhance the growth of NAPL fingers, indicating that pump-and-treat systems by extracting contaminated groundwater might enhance NAPL dissolution fingering and lead to less uniform dissolution fronts.

1. Introduction

In the field of contaminant hydrology, both the land contamination and the land remediation problems are often encountered. Land contamination is known as the distribution of chemical and pollutants on land sites, while land remediation is known as the cleanup of chemical and pollutants on land sites that causes health concerns to humans and the environment. When nonaqueous phase liquids (NAPLs), such as trichloroethylene, ethylene dibromide, benzene, toluene and so forth (Miller et al., 1990), are released to groundwater, they can reside in the form of disconnected ganglia or blobs as residual saturations within the pores of porous media. This process belongs to the land contamination problem. Some NAPLs (e.g. trichloroethylene and ethylene dibromide) are heavier than water, but others (e.g. benzene and toluene) are lighter than water. Although their solubilities in groundwater are very low, the effect of such NAPLs on the quality of groundwater resources is severe because of their relatively high toxicity. Thus, it is necessary to remove such NAPLs from the contaminated land site. This process belongs to the land remediation problem, which is the main focus of this paper.

To develop effective and efficient methods for removing the residual NAPLs from the contaminated land sites, the

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0169-7722/$ – see front matter
doi:10.1016/j.jconhyd.2012.07.001

detailed transport mechanism of NAPLs in fluid-saturated porous media has been studied, both experimentally and analytically, during the past two decades (Geller and Hunt, 1993; Imhoff et al., 1994, 1996, 2002, 2003a, 2003b; Miller et al., 1990, 1998; Powers et al., 1994; Seyedabbasi et al., 2008; Soerens et al., 1998; Willson et al., 1999). Notable achievements from existing laboratory experiments are as follows: (1) mass transfer rates between a NAPL and an aqueous phase liquid can be determined in a quantitative manner; (2) the fingering phenomena of NAPL dissolution fronts have been observed at the laboratory (i.e. centimeter) scale; and (3) the linear stability theory has been employed to derive the critical condition that can be used to assess the instability of NAPL dissolution fronts in fluid-saturated porous media. For example, the Zhao number (see Appendix A for a detailed discussion), which is a comprehensive dimensionless number, was proposed to represent the three major controlling mechanisms simultaneously taking place in a NAPL dissolution system. Based on the linear stability theory, a NAPL dissolution system may physically have three different kinds of states (Imhoff and Miller, 1996; Zhao et al., 2008c, 2010a): in the supercritical state NAPL dissolution fingering occurs, but it does not occur in the subcritical state. The neutral condition (or state) is just the interface between the two. Correspondingly, three kinds of the Zhao numbers, namely the subcritical Zhao number, the critical Zhao number and the supercritical Zhao number, can be used to represent these three different kinds of states in the NAPL dissolution system. As a direct result of these achievements, both mathematical and computational models (Imhoff and Miller, 1996; Miller et al., 1998; Zhao et al., 2010a) were developed to simulate the morphological evolution of NAPL dissolution fronts in fluid-saturated porous media. Nevertheless, to the best of the authors' knowledge, the existing computational models are mainly limited to either a square domain or a rectangular domain, so that it is necessary, in this paper, to investigate the effects of different domain shapes on the morphological evolution of NAPL dissolution fronts in fluid-saturated porous media.

It needs to be pointed out that NAPL dissolution fingering requires regions of continuous NAPL saturation distribution (in the form of disconnected ganglia or blobs as residual within the pores of the porous medium) and has been observed in experiments with length scales of 7 cm and larger in the mean flow direction (Imhoff et al., 2003a, 2003b). This requirement is unlikely to be satisfied for most two-dimensional experimental systems considered in the laboratory where a small amount of NAPL is spilled (Chen and Jawitz, 2008; DiFilippo et al., 2010). However, as demonstrated previously (Christ et al., 2006, 2009; Gerhard et al., 2007; Parker and Park, 2004), for large NAPL spill sites, continuous regions of residual NAPL occurred so that the above-mentioned requirement can be met. For example, in the work of Parker and Park (2004) a NAPL spillage event resulted in vertical fingers that on average were 30 cm in diameter. These fingers primarily contained residual NAPL. On the other hand, since most grid blocks used in current field-scale simulations were on the order of 30–50 cm (in the x and y dimensions), by necessity NAPL-contaminated grid blocks only represent continuous regions of NAPL (often residual) that exceed the 7 cm scale. As a result, these simulations might ignore NAPL dissolution fingering. It is a sub grid-block process that is not accounted for. The local (grid-block scale) rate of NAPL dissolution may not be important for many field problems, since the bypassing of water around NAPL-contaminated zones (Parker and Park, 2004) is the slowest process limiting NAPL dissolution into surrounding groundwater. However, recent simulations indicate that for some systems local NAPL dissolution rates are important in heterogeneous media (Maji and Sudicky, 2008). For such systems, NAPL dissolution fingering may be important. Thus, an understanding of NAPL dissolution fingering may be important for developing innovative remediation strategies and technologies to some NAPL contaminated groundwater systems.

In addition to NAPL dissolution fingering, preferential flow within NAPL contaminated zones can be also caused by either medium heterogeneity (Maji and Sudicky, 2008) or variations in NAPL saturation, which in nature are not uniform in space (Grant and Gerhard, 2007; Zhang et al., 2007). Medium heterogeneity within NAPL-contaminated zones will result in a variation in aqueous-phase permeability. Some of this variation is associated with the variation in intrinsic permeability caused by the medium heterogeneity alone, while some is associated with the variation in NAPL saturation, which alters the relative permeability. Nevertheless, the mechanism of the preferential flow caused by NAPL dissolution fingering is different from that caused by medium heterogeneity. From the physical point of view, the former is considered as an emerging phenomenon due to the instability of a nonlinear system (Chadam et al., 1986, 1988; Chen and Liu, 2002, 2004; Chen et al., 2009; Ortoleva et al., 1987; Renard et al., 1998; Zhao et al., 2008a, 2008b, 2008c, 2009, 2010a, 2010b), while the latter is considered as the conventional phenomenon of a nonlinear system (Alt-Epping and Smith, 2001; Maji and Sudicky, 2008; Ormond and Ortoleva, 2000; Raffensperger and Garven, 1995; Schafer et al., 1998; Steefel and Lasaga, 1990, 1994; Yeh and Tripathi, 1991).

Since the domain of a NAPL dissolution system in the real world may have many different shapes, it is difficult, if not impossible, to use a typical domain shape to represent all computational domains of NAPL dissolution systems encountered in the real world. However, for the purpose of investigating the effect of a domain shape on the interesting features associated with NAPL dissolution fingering, it is feasible to use a generic model of a specific shape (that is, to some extent, an artificial system) in the computational simulation, as long as some fundamental flow characteristics associated with irregular domains can be reasonably reflected in the generic model. On the other hand, due to the versatility and robustness of computational methods, any complicated domain shapes can be realistically simulated if their details can be precisely given. Compared with rectangular and square domains that are widely used in the previous studies (Imhoff and Miller, 1996; Miller et al., 1998; Zhao et al., 2010a), some important flow characteristics associated with irregular domains are as follows (Maji and Sudicky, 2008; Zhang et al., 2007). First, the pore-fluid flow in an irregular domain of a subcritical Zhao number is multi-directional (i.e. two-dimensional for a two-dimensional problem domain and three-dimensional for a three-dimensional problem domain) rather than unidirectional, just as what was observed in a rectangular or square domain of a subcritical Zhao. Second,