Journal of Colloid and Interface Science 368 (2012) 558–577

Contents lists available at SciVerse ScienceDirect

Journal of Colloid and Interface Science

www.elsevier.com/locate/jcis

Contact line extraction and length measurements in model sediments and sedimentary rocks

Elena Rodriguez *, Maša Prodanović, Steven L. Bryant

Department of Petroleum and Geosystems Engineering, University of Texas at Austin, 1 University Station C0300, Austin, TX 78712, USA

ARTICLE INFO

Article history:
Received 28 May 2011
Accepted 28 October 2011
Available online 10 November 2011

Keywords:
Contact line length
Interfacial area
Colloid retention
Drainage
Imbibition
Level set method
X-ray images
Model sediments

ABSTRACT

The mechanisms that govern the transport of colloids in the unsaturated zone of soils are still poorly understood, because of the complexity of processes that occur at pore scale. These mechanisms are of specific interest in quantifying water quality with respect to pathogen transport (e.g. *Escherichia coli*, *Cryptosporidium*) between the source (e.g. farms) and human users. Besides straining in pore throats and constrictions of smaller or equivalent size, the colloids can be retained at the interfaces between air, water, and grains. Theories competing to explain this mechanism claim that retention can be caused by adhesion at the air–water-interface (AWI) between sediment grains or by straining at the air–water–solid (AWS) contact line. Currently, there are no established methods for the estimation of pathogen retention in unsaturated media because of the intricate influence of AWI and AWS on transport and retention. What is known is that the geometric configuration and connectivity of the aqueous phase is an important factor in unsaturated transport. In this work we develop a computational method based on level set functions to identify and quantify the AWS contact line (in general the non-wetting–wetting–solid contact line) in any porous material. This is the first comprehensive report on contact line measurement for fluid configurations from both level-set method based fluid displacement simulation and imaged experiments. The method is applicable to any type of porous system, as long as the detailed pore scale geometry is available. We calculated the contact line length in model sediments (packs of spheres) as well as in real porous media, whose geometry is taken from high-resolution images of glass bead packs and sedimentary rocks. We observed a strong dependence of contact line length on the geometry of the sediment grains and the arrangement of the air and water phases. These measurements can help determine the relative contribution of the AWS line to pathogen retention.

Published by Elsevier Inc.

1. Introduction

Particles of colloidal size (effective diameters between 0.01 and 10 μm) are naturally present in the subsurface. Some examples include humic materials, silicate clays and mineral precipitates, and viruses and bacteria. These colloid particles themselves can be contaminant (bacteria and viruses) or they can act as carriers of contaminants such as pesticides or heavy metals [1]. The presence and transport of colloids in the subsurface strongly affect ground water quality and consequently the transport and retention mechanisms of these particles are of specific interest in quantifying water quality with respect to pathogen transport (e.g. *Escherichia coli*, *Cryptosporidium*) between the source (e.g. farms) and human users. In a completely different, but not less important field, inorganic colloids, such as clay particles, can cause problems in oil reservoirs, affecting the reservoir properties of sandstones. These particles can move within the reservoir due to drag forces during oil and gas production. This phenomenon is known as fines migration and consists of the release of the fine particles from the porous media, their movement with the flow of permeate, and eventually their capture within the porous medium or their path out of the medium. Migration and capture in oil reservoirs can cause a reduction in permeability and therefore a decline in oil production.

In the unsaturated zone of the sediments, particles can be retained at the interfaces between air, water, and grain. This retention is in addition to straining at pore throats and constrictions of smaller or equivalent size.

Because of the complexity of processes at the pore scale, the mechanisms that govern retention in the unsaturated zone are still poorly understood. Theories competing to explain this mechanism claim that retention can be caused by adhesion at the air–water-interface (AWI) between sediment grains [2,3] or by straining at the air–water–solid (AWS) contact line [4,5]. At this time, the discussion about the relative contributions of AWI and AWS to retention which started several years ago is still unsettled. Another

---

* Corresponding author. Permanent address: 1200 Post Oak Blvd., Apt. 1613, Houston, TX 77056, USA.

E-mail addresses: erodriguez@alumni.utexas.net (E. Rodriguez), masha@ices.utexas.edu (M. Prodanović), steven_bryant@mail.utexas.edu (S.L. Bryant).

0021-9797/$ - see front matter Published by Elsevier Inc.
doi:10.1016/j.jcis.2011.10.059

factor that makes the particles susceptible to retention at these interfaces is their affinity for the aqueous phase and therefore the water saturation. Also important are factors like pH or ionic strength of the particle solution. For example, Torkzaban et al. [6] investigated the factors that control the attachment to the AWI in column experiments using solutions of bacteriophages at different pH and ionic strengths. The experiments showed that retention at AWI and SWI (solid–water-interface) increased as the pH decreased and that electrostatic interactions were more important than hydrophobicity regarding attachment to the AWI. On the other hand, Gao et al. [7] credit capillary and friction forces rather than electrostatic (DLVO) forces to be responsible for the retention of colloids at the AWmS.

More recently, Bridge et al. [8] studied the movement of colloids during drainage in quartz sands and observed colloid mobilization by AWI while the AWS contact plays the part of fixing the colloids to the SWI.

Currently, there are no established methods for the estimation of particle retention in unsaturated media because of the intricate influence of AWI and AWS on transport and retention. The geometric configuration and connectivity of the aqueous phase and air phase are clearly important factors in unsaturated transport. But reliable quantitative estimates of the specific interfacial area are still difficult to obtain: measurements with interfacial tracers typically include contribution from wetting films in drained pores [9,10], and direct observation (e.g. from epoxy-filled sections [11] or from high-resolution X-ray images [12,13]) is tedious to acquire. No estimates of lengths of AWS contact have been reported to date.

In this paper we quantify of the length of the air–water–solid (in general non-wetting–wetting–solid) contact line in simple geometries and granular materials. When colloidal retention data is available (expressed for example as number of colloidal particles per volume of column effluent) the length of the contact line and the interfacial area between wetting and non-wetting phases can be used to make predictions about where the colloidal size particles are trapped when compared with experimental visualizations, and thus improve our understanding of the underlying mechanisms.

We used a novel computational, level set method based, progressive quasi-static algorithm (LSMPQS) to reveal the configuration of the air–water–solid (AWS) contact lines. LSMPQS tracks the pore scale motion of interfaces assuming capillary forces are dominant [14]. It has been implemented to compute the location of an interface between two immiscible fluids confined by arbitrary solid surfaces. Thus the method implicitly determines the location of contact lines as the intersection of any pair of interfaces (e.g., the intersection of the wetting–non-wetting interface with the wetting–solid interface) as a function of applied capillary pressure. The volume fraction occupied by water, the total interfacial areas, and the contact line length are recorded for each configuration.

While energy, mass and momentum conservation equations for the "common lines" have been developed [15,16] and the importance of contact lines in the modeling of multiphase flow in porous media has been explored, [17,18] to our knowledge, this is the first comprehensive work on quantifying contact line lengths in disordered porous media. McClure et al. [19] report the ability to measure contact lines but their focus is primarily on interface areas and curvatures.

The contact lines have been identified and computed in model sediments (random packs of spheres). We validate these computations using fluid configurations extracted from high resolution images of glass beads packs and consolidated rock formations (Fontainebleau sandstone and sucrosic dolomite).

2. Methods

2.1. Level set method

Measuring the contact line length requires detailed knowledge of wetting and non-wetting interface positions in the granular medium under investigation. We use both LSMPQS simulation and microtomography images as a source of such knowledge. LSMPQS algorithm [14] determines the geometry of capillarity controlled fluid configurations and thus readily provides pore scale interfacial areas (wetting/non-wetting, wetting/solid, non-wetting/solid). The fluid interfaces are confined by solid surfaces which correspond to the grains in the porous medium. The contact lines exist at the intersection of these interfaces with grain surfaces. Fig. 1a shows non-wetting phase (air) displacing wetting phase (water) between two solid grains. The point contacts at the intersection between fluid–fluid interface and solid in the 2D schematic will become contact lines in 3D.

The level set method is a numerical method for propagating interfaces [20]. The fluid locations are defined by an arbitrary function $\varphi(x)$, where x is a position vector, whose value is zero at the interface between the two fluids, less than zero for the non-wetting phase and larger than zero for the wetting phase. This interface is allowed to move normal to itself with a velocity which defines the physics of the problem. Its motion is governed by the following equation:

$$\varphi_t - F|\nabla\varphi| = 0 \tag{1}$$

Therefore the physics of the problem are given by the definition of F. In our porous medium application, changes in capillary forces are driving the displacement of one fluid by another. Thus F is defined as:

$$F = P_c - \sigma\kappa \tag{2}$$

where P_c is the capillary pressure, σ is the interfacial tension between fluids and κ is twice the mean curvature of the interface. For our application F is defined as follows:

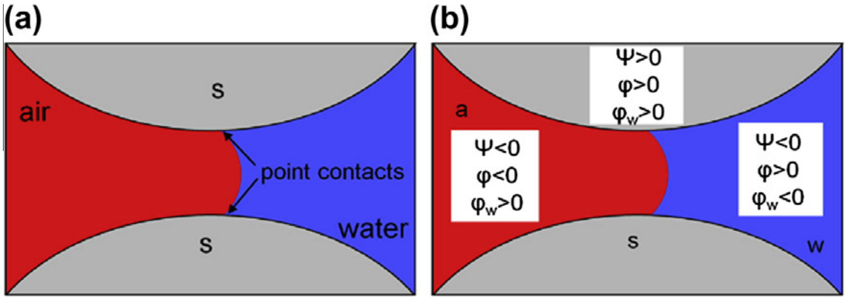

Fig. 1. (a) Displacement of wetting phase (water) by non-wetting (air) in a simple pore throat (s = solid). (b) Level set function for the non-wetting fluid (φ), wetting fluid (φ_w) and solid (ψ) phases.