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Numerical study of the effects of contact angle and viscosity ratio on the dynamics of snap-off through porous media

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ABSTRACT

Snap-off is a pore-scale mechanism occurring in porous media in which a bubble of non-wetting phase displacing a wetting phase, and vice-versa, can break-up into ganglia when passing through a constriction. This mechanism is very important in foam generation processes, enhanced oil recovery techniques and capillary trapping of CO_2 during its geological storage. In the present study, the effects of contact angle and viscosity ratio on the dynamics of snap-off are examined by simulating drainage in a single pore-throat constriction of variable cross-section, and for different pore-throat geometries. To model the flow, we developed a CFD code based on the Finite Volume method. The Volume-of-fluid method is used to track the interfaces. Results show that the threshold contact angle for snap-off, i.e. snap-off occurs only for contact angles smaller than the threshold, increases from a value of 28° for a circular cross-section to 30–34° for a square cross-section and up to 40° for a triangular one. For a throat of square cross-section, increasing the viscosity of the injected phase results in a drop in the threshold contact angle from a value of 30° when the viscosity ratio $\overline{\mu}$ is equal to 1 to 26° when $\overline{\mu} = 20$ and down to 24° when $\overline{\mu} = 20$.

1. Introduction

Multiphase fluid flow in porous media is encountered in many practical engineering problems, including oil, water and gas flow in petroleum reservoirs, and storage of Carbon Dioxide (CO_2) in deep underground aquifers. There are two types of displacement which can take place in two-phase systems: drainage, in which the wetting phase (water, in this work) is displaced by a non-wetting phase (typically a gas, for example CO_2), and imbibition, in which the wetting phase is adsorbed into the porous medium and displaces the resident non-wetting phase. A dominant pore-scale mechanism occurring when a non-wetting phase is injected into a reservoir predominanly occupied by a wetting phase, and vice versa, is the break-up of the injected phase into several ganglia when passing through a constriction. This mechanism is called "snap-off" (Gauglitz and Radke, 1990; Kovscek and Radke, 1996; Ransohoff et al., 1987; Roof et al., 1970; Rossen, 2000). It is relevant to foam generation processes and capillary trapping of oil or CO_2 bubbles during enhanced oil recovery or geological storage of CO_2. Several studies have been conducted to analyze the snap-off mechanism in order to establish a criterion for its occurrence. The first quasi-static criterion was derived by Roof et al. (1970) for circular pores and for perfectly wetting conditions ($\theta = 0°$). The criterion states that snap-off occurs when the capillary pressure at the bubble front in the unconstricted pore becomes less than the local capillary pressure at the throat, i.e. when the following inequality is satisfied:

$$\frac{2}{R_p} \leq \frac{1}{R_t} + \frac{1}{R_{zt}}, \tag{1}$$

where R_p and R_t are the pore and throat radii and R_{zt} is the longitudinal radius of curvature of the throat. In Eq. (1), the left hand side is the mean curvature of the bubble front in the unconstricted section of the pore while the right hand side is the local curvature of the throat. Ransohoff et al. (1987) extended Roof's criterion to variable cross-sections as follows:

$$\frac{\widetilde{C}_p}{R_p} \leq \frac{1}{\widetilde{R}_t} + \frac{1}{R_{zt}}, \tag{2}$$

where the coefficient $\widetilde{C}_p$ depends on the shape of the cross-section ($\widetilde{C}_p = 2$ for circular, 1.89 for square and 1.77 for triangular), $\widetilde{R}_t$ is the radius of the largest inscribed circle at the throat and the r.h.s. is the critical curvature for snap-off at the throat, corresponding to the point of instability where the curvatures at two corners of the cross-section meet. For long enough throats, the above criterion reduces to

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$$R_p \geq \widetilde{C}_p \widetilde{R}_t. \tag{3}$$

This is a purely geometric criterion stating that snap-off occurs when the contraction ratio CR, defined as

$$CR = \frac{R_p}{R_t}, \tag{4}$$

satisfies certain conditions. However, geometry-constrained snap-off, governed by Roof's criterion, is not the only mechanism for snap-off to occur (Rossen, 2003). Considering a capillary channel with sinusoidal shape, when the invading fluid becomes continuous within the channel, its break-up is determined by the imbalance between the pressure critical values at the necks and pores (Beresnev et al., 2009). To this extent, Beresnev and Deng (2010) developed a theory of fluid break-up in sinusoidally constricted capillary channels. Their formulation reduces to the condition for Rayleigh instability as a limiting case. Deng et al. (2014) used the latter model to study the snap-off of CO_2 in capillary channels of such sinusoidal profile. They considered capillary channels with different wavelenghts but fixed contraction ratio. They then observed that snap off can occur even in capillary channels which do not meet Roof's criteria. Hence, they proposed a new criterion of the form

$$\frac{\widetilde{C}_p}{\widetilde{R}_p} + \frac{1}{R_{zp}} \leq \frac{\widetilde{C}_t}{\widetilde{R}_t} + \frac{1}{R_{zt}}, \tag{5}$$

where R_{zp} is the longitudinal radius of curvature of the pore. Raeini et al. (2014) investigated the existence of a threshold contraction ratio for snap-off for a single star-shaped pore-throat system of different aspect ratios AR

$$AR = \frac{L_t}{R_p}, \tag{6}$$

where L_t is the length of the throat. Finally Armstrong et al. (2016) used Density Functional Hydrodynamics (DFH) tools to study geometry-constrained snap-off in pore doublets and simple systems of pores, demonstrating consistency of simulation results with theoretical criteria. In particular, they compared the curvature at the leading interface measured from the numerical simulations against its theoretical value at the moment of snap-off from Roof's model. They observed slight discrepancy between these values due to the fact that theoretical models assume quasi-static conditions while inertial effects are present in numerical simulations. However, they also observed that this discrepancy tends to decrease with increasing grid resolution.

However, the last numerical studies assumed perfectly wetting behaviour between the two fluids, i.e. $\theta = 0°$. Little effort has been devoted to quantifying the influence of contact angle on the occurrence of snap-off. Yu and Wardlaw (1986) carried out experiments under quasi-static conditions on a single pore-throat system of square cross-section. They found that the critical contraction ratio for snap-off increases only slightly from 1.5, when θ is equal to zero, to 1.75, when $\theta = 55°$, however above $\sim 70°$ snap-off never occurs. Pore-network studies (Blunt et al., 1997; Mogensen and Stenby, 1998) indicated that snap-off is inhibited for $\theta > 45°$ when throats have a square cross-section.

In the present study, the effects of contact angle and viscosity on the dynamics of snap-off are examined. The dimensionless quantities describing the flow that will be used in the following are the Reynolds number Re, the capillary number Ca and the viscosity ratio defined as:.

$$Re = \frac{\rho v D}{\mu}, \tag{7a}$$

$$Ca = \frac{\mu v}{\sigma}, \tag{7b}$$

$$\overline{\mu} = \frac{\mu_{nw}}{\mu_w}, \tag{7c}$$

where v is the velocity, ρ and μ are the fluid's density and viscosity, D is the diameter of the pipe and σ is the interfacial tension. The study is conducted by simulating drainage in a single pore-throat constriction of variable cross-section and for different pore-throat geometries. To model the flow, we developed the C++ in-house code *interpore3d* which solves the governing equations by means of the Finite Volume (FV) method. The numerical method is described in Section 2. Simulation results of benchmark problems for model validation are presented in Section 3. These include the classic static drop problem and simulations of imbibition in a circular pipe for different flow conditions. Finally, simulation results of snap-off are presented in Section 4.

2. Numerical method

The method consists of three main components: an interface-tracking algorithm, a model for the surface tension forces and a solver for the incompressible Navier–Stokes (NS) equations.

2.1. The interface-tracking algorithm

The interfaces are tracked using the Volume-of-Fluid (VOF) method by Hirt and Nichols (1981). The VOF method is a volume-tracking method for the representation of the interfaces in interfacial flow problems, in which the fluids are marked and tracked by means of a volume fraction, also called indicator function. In a VOF-FV framework, the indicator function α is defined for each cell as the ratio between the volume of fluid 1 contained within the cell, V^α, and the volume of the cell V as

$$\alpha = \frac{V^\alpha}{V}. \tag{8}$$

This means that the indicator function is bounded between 0 and 1 as follows

$$\alpha = \begin{cases} 1, & \text{if the cell is filled with fluid 1,} \\ 0, & \text{if the cell is filled with fluid 2,} \\ 0 < \alpha < 1, & \text{if there is an interface within the cell.} \end{cases} \tag{9}$$

Starting from a known initial distribution, the volume fraction is updated in time by solving the following advection equation

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = \alpha \nabla \cdot \mathbf{u}, \tag{10}$$

where t is time and $\mathbf{u}$ is the velocity vector. Advection is done through operators-splitting, i.e. the interface is advanced in time with three independent sweeps along each of the three directions, where the order of the sweeps is alternated at each time step to ensure better stability. We employed the Piecewise Linear Interface Calculation (PLIC) method by Youngs (1982) to solve Eq. (10) numerically. In the PLIC method, the interface is mathematically described as a planar surface defined by equation

$$\mathbf{n} \cdot \mathbf{x} - \beta = 0, \tag{11}$$

where β is a constant and $\mathbf{n}$ is the interface unit normal vector pointing outwards from fluid 1:

$$\mathbf{n} = -\frac{\nabla \alpha}{|\nabla \alpha|}. \tag{12}$$

The minus sign in Eq. (12) comes from the choice of the normal pointing direction. Discretization of the gradient operator in Eq. (12) is done using a 27 points-stencil Finite Difference scheme, while determination of the constant β is done by matching the interface truncated volume $V(\mathbf{n}, \beta)$ (the volume ABCDIJKL in Fig. 1) to the actual fluid volume V^α contained in the cell using Brent's method (Press et al., 1996). A useful formula for the truncated volume is given by Gueyffier et al. (1999). Further detail on the PLIC algorithm can be found in Kothe et al. (1996) and Rider and Kothe (1998).