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Self-driven penetration of droplets into non-wetting capillaries

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ABSTRACT

This is a successive study to our previous study published in this journal. In the present study, a further numerical study on the penetration of a droplet into non-wetting capillaries is carried out by using many-body dissipative particle dynamics (MDPD). The simulation results show the outer (outside of the capillary) and inner (inside of the capillary) curvatures of the droplet can cause two Laplace pressures. The difference between these two pressures forms a net pushing force which directly drives the droplet flowing into the non-wetting capillary. We give a detailed analysis on how the outer and inner curvatures change during the penetration process. To further show the effect of the Laplace pressure difference on the droplet movement, we also simulate a new droplet/capillary/film system. In this system, the droplet and liquid film are placed at both ends of a prefilled capillary. It is very interesting to find that the droplet penetrates even faster in lyophobic capillaries over lyophilic ones, and the spontaneous penetration does not pose any wettability restriction which is different from previous study in literatures. The present work is expected to provide new ideas for designing microfluidics or nanofluidics devices by utilizing the driving force from the droplet itself.

1. Introduction

Capillarity is omnipresent in nature and plays a vital role in different processes, such as transport of liquids in soil and plants and directional water collection on wetted spider silk [1]. It also finds a wide range of applications in industry. For example, it can be used for capillary force lithography at nanoscale [2]. Moreover, the application of capillary force in the formation of adaptive graphene gel films, has also been reported recently [3]. As a unique capillary process, the spontaneous penetration of a liquid droplet into hydrophobic (or non-wetting) capillaries was theoretically elucidated by Marmur in 1988 [4], and then it has motivated a large number of experimental and computational studies [5–8]. Schebarchov and Hendy [5,6] proposed a model to calculate the change of surface energy based on different interactions between droplets and capillaries. In fact, their model is an extension of the Lucas-Washburn model [9,10] and can be used to predict the spontaneous uptake of droplet into non-wetting capillaries. Willmott et al. [7] experimentally found that the penetration rate of smaller liquid droplets is greater than that of larger ones. Piroird et al. [8] found that a slight perturbation on an unstable droplet in a completely non-wetting capillary can cause the droplet extraction from the capillary, and the droplet velocity increases with extraction time. Chen and coworkers carried out a series of studies on spontaneous [11] and forced [12] liquid flow in capillaries with MDPD method. In these previous studies, the Laplace pressure was considered as the driving force behind the spontaneous uptake but without further analysis. In this paper, we aim to show how the curvatures of both sides of the droplet change and affect the penetrating process numerically.

The present simulations were carried out by using a coarse-graining and particle-based numerical method, MDPD method, which is widely used for studying complex fluid systems with free liquid/vapor interface at mesoscale [11–20]. For generality reason [15], we don't specify the materials of the liquid, it could be water or oil or others. The same strategy is also applied to the solid surface of capillaries, which also could be any solid material. The only requirement in the simulations is the related wettability formed by the interaction between the droplet and capillary. Also, we use words "lyophilic" and "lyophobic" to describe the wettability instead of "hydrophilic" and "hydrophobic" by following this generality strategy. To validate the critical spontaneous uptake condition proposed by previous studies [4–7], we have performed a series of simulations, a good agreement has been achieved, as shown in our previous work [16]. All the simulation setting are the same with our previous study [16]. In this work and ref. [16], the capillaries are constructed by the following steps: First, 240,000 homoge-

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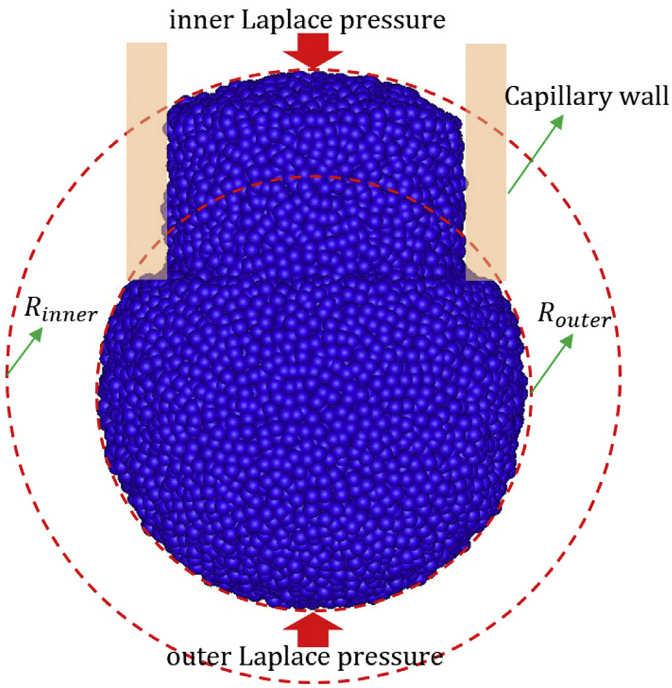

Fig. 1. The schematic diagram for the spontaneous penetration of a droplet into lyophobic capillaries. R_{outer} and R_{inner} are the dynamical radii of the two meniscuses of the droplets.

neous particles are placed in regularly in a $20 \times 50 \times 20$ calculation box; then all the particles in the calculation box are relaxed for enough time to reach a stabilized state when the particle number density and temperature are distributing evenly. Second, by proper programming, various sizes of capillaries can be cut from this well-stabilized raw material.

The remainder of this paper is organized as follows. In Section 2, a theoretical basis regarding to spontaneous uptake of droplet into non-wetting capillaries is provided; then the simulation results are presented in Section 3; at last we summary our work in the conclusions in Section 4.

2. Theoretical background

Here we give a theoretical explanation on the spontaneous uptake of droplet into non-wetting capillaries. This time we focus on the curvature change of the inner and outer meniscus of the droplet, this is more intuitionistic than our previous analysis from a force balance viewpoint [16]. When a droplet comes into contact with the capillary with a very slow initial velocity, some liquid from the droplet will squeeze into the capillary and then a meniscus will form inside the capillary. If the capillary wall is lyophilic to the droplet (with contact angle $\theta_s < 90°$), the meniscus will be in a concave shape. The Laplace pressure of the meniscus will act as a pulling force to drag the droplet into the capillary. On the contrary, if the capillary wall is lyophobic to the droplet (with contact angle $\theta_s > 90°$), a convex meniscus with a radius R_{inner} will form, as shown in Fig. 1, and the Laplace pressure will push the liquid out of the capillary. Because the outer part of the droplet is always convex with a radius R_{outer}, an outer Laplace pressure will tend to push the liquid into the capillary, as shown in Fig. 1. Then the flow direction of the droplet will depend on which Laplace pressure is larger, the inner or outer one. According to the studies in ref. [4–7], the requirement for spontaneous penetration of a droplet into the lyophobic capillary is described as follows:

$$R_d < -R_t / \cos\theta_s \tag{1}$$

where R_d is the initial radius of the droplet, R_t is the radius of the capillary and θ_s is the contact angle of the droplet on the capillary wall.

3. Results and discussion

3.1. Penetration of a droplet into lyophobic capillaries

In this work, we assume the length scale is small enough where the interfacial effect dominates, it could be in a mesoscale from dozens of nanometres to hundreds of microns. In this length scale

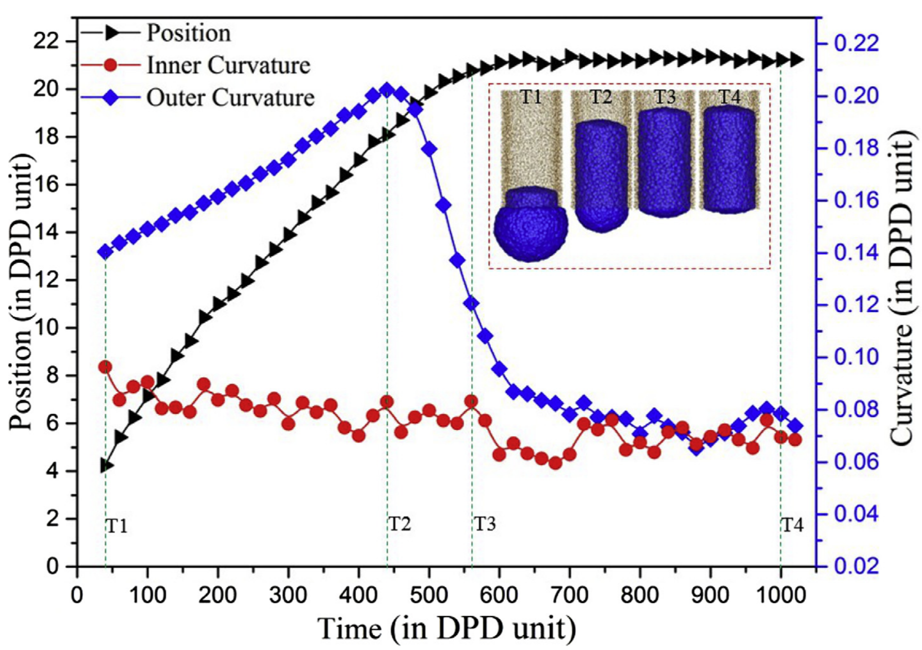

Fig. 2. Time-dependent variation of the inner and outer curvatures and the position of the inner meniscus front. The inset shows snapshots at four characteristic moments. In this case, $R_d = 7$, $R_t = 5$ and the static contact angle $\theta_s = 108.5°$.