# *Supporting Information*

# A Many-Body Dissipative Particle Dynamics Study of Fluid-Fluid Spontaneous Capillary Displacement

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## I. Computational details

***Three-phase static contact angle* ($\theta_{03}$).** The $\theta_{03}$ calculation is illustrated employing a capillary of radius $r$ = 10 (see Figure 1 in the main text). The simulation process involves the following steps: First, a 32.5 × 22 × 22 bulk of fluids ($\rho$ = 6.0) with 95269 particles is placed in a 37.5 × 22 × 22 simulation box, and periodic boundaries are applied in all three dimensions. Vacuum spaces are placed to both ends of the simulation box along $x$ axis to avoid possible interactions across the boundary. After equilibration in NVE ensemble for 1000 MDPD time units, the homogeneous system is fully relaxed and ready for partition. As is depicted in Figure 1c, Particles to the left with $-2.5 < x < 0$ are classified as fluid constituting the wall, which seals the left entrance of the capillary. Particles with $0 \le x \le 30$ are divided into two main region, i.e. a cylinder ($r$ = 10) sharing axis with the cuboid and the remained part. Particles in the remained part construct the capillary, and particles in the cylindrical region are further divided into a FA column ($0 \le x < 12.5$), an FB column ($12.5 \le x \le 25$), a piston ($25 \le x \le 27.5$), and that to be deleted ($27.5 < x \le 30$).

$$\mathbf{F}_S = k_S(\mathbf{r}_i(t) - \mathbf{r}_i(0)) \tag{S1}$$

Once the system is ready, following eq S1, the pinning forces $\mathbf{F}_S$ are applied to the capillary and wall particles,[1] making them equilibrate at their initial position, and the piston particles are only allowed to move in a rigid entity along $x$ direction. In such condition the system is equilibrated in NVE ensemble first for 1000 MDPD time units, followed by 1000 MDPD time units for data production (Figure 1d).

To extract the $\theta_{03}$, only positions of FA particles is needed, since there is no detachment at the interface. As is documented in our previous reports,[2,3] the fluid column is divided into concentric cylindrical shells away from the capillary axis with an interval $\Delta r = 1$ for $r = 10$, 15, 20, 25, while $\Delta r = 0.5$ for $r = 5$ case. The position of interface is obtained by doubling the distance of center of mass of FA in this layer to the left entrance of capillary. Based on the averaged position of each layer, a fitted circle would intersect with the capillary boundary, where the $\theta_{03}$ is easily extracted. The uncertainty of the contact angle thus extracted is within 20%.

***Spontaneous capillary displacement.*** For system construction, a 110 × 22 × 22 bulk of fluids ($\rho = 6.0$) with 297815 particles is placed in a 120 × 22 × 22 simulation box, and periodic boundaries are applied in all three dimensions. Vacuum spaces are placed to both ends of the simulation box along $x$ axis to avoid possible interactions across the boundary. After equilibration in NVE ensemble for 1000 MDPD time units, the homogeneous system is fully relaxed and ready for partition. Particles to the left with $-40 < x < -10$ are classified as fluid constructing FA reservoir, while those to the right with $30 < x < 40$ constructing the FB reservoir. Between the FA and FB reservoirs, particles with $-10 \leq x \leq 30$ are classified into a coaxial fluid cylinder with $r = 10$, thus the remained capillary has a slit of round-shaped cross-section. The fluid cylinder in capillary is mainly composed of FB, and a $\theta_{03}$ is pre-formed, which means there is a FA meniscus formed beforehand with the arc bottom aligned to the left entrance of the capillary, whose importance is illustrated in the Figure 7 in the main text.

Once the system is ready, following eq S1, the pinning forces are applied to the capillary and FA particles,[1] making them equilibrate at their initial positions, and the FB particles are left free to relax. This pre-equilibration lasts for 100 MDPD time units, and in a subsequent 100 MDPD time units, the capillary and FB particles are pinned with the FA particles being

free to relax. Thereafter, the pinning force acting on either FA or FB particles are removed, and then the spontaneous capillary displacement begins. The spontaneous capillary displacement process lasts for 400 MDPD time units, and the motions of FA/FB interface as well as other layers are recorded accordingly, which are used for the calculation of $\theta_{d3}$.

## II. Supplementary tables

**Table S1.** Interfacial tension $\gamma_{AB}$ for different fluid-fluid interaction parameter $A_{AB}$.

| $A_{AB}$ | $\gamma_{AB}$ | $A_{AB}$ | $\gamma_{AB}$ |
|---|---|---|---|
| -40 | 0±0.05 | -20 | 11.42±0.02 |
| -37.5 | 0±0.02 | -17.5 | 12.18±0.04 |
| -35 | 2.32±0.03 | -15 | 12.85±0.06 |
| -32.5 | 3.68±0.03 | -12.5 | 13.32±0.03 |
| -30 | 6.45±0.02 | -10 | 13.84±0.02 |
| -27.5 | 8.03±0.01 | -7.5 | 13.84±0.03 |
| -25 | 9.30±0.04 | -5 | 14.60±0.18 |
| -22.5 | 10.45±0.05 | -2.5 | 14.56±0.12 |

**Table S2.** Slip length $b$ for different solid-liquid interaction parameter $A_{SL}$.

| $A_{SL}$ | $b$ | $A_{SL}$ | $b$ |
|---|---|---|---|
| -40 | 0±0.00 | -27.5 | 0.41[a] |
| -37.5 | 0.05±0.01 | -25 | 0.55±0.05 |
| -35 | 0.1±0.01 | -22.5 | 0.69±0.07 |
| -32.5 | 0.15±0.01 | -20 | 0.95±0.03 |
| -30 | 0.27[a] | -17.5 | 1.30±0.05 |

[a] Data acquired from the fitting curve with other data points

**Reference**

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3. Chen, C.; Lu, K.; Zhuang, L.; Li, X.; Dong, J.; Lu, J. Effective Fluid Front of the Moving Meniscus in Capillary. *Langmuir* **2013**, *29*, 3269-3273.