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Volume of Fluid based study of the three phase dynamic contact line in wetting of the nanometric rough micro-channels

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The precise representation of molecular motion near the three-phase dynamic contact line remains a significant research challenge [1], with substantial practical implications [2]. We investigate the two-phase flow in a pressure driven micro channel (width ~ 1μm - 10μm) having a nanometric surface roughness. The two phases are separated by an interfacial layer with surface tension, that meets the moving pipe wall, hence, a three phase dynamic contact line is formed. Numerical simulations are conducted by solving the 2D two-phase Navier-Stokes equation using the Basilisk flow solver. The Volume-of-Fluid method is employed to capture the interface, and the surface tension force is computed using the Continuous Surface Force method. Additionally, curvature calculation is done using height functions. To address the influence of surface roughness, we develop a hybrid Volume-of-Fluid coupled embedded boundary solver. This hybrid solver enables the imposition of a contact angle on arbitrarily shaped solids. We explore scenarios where (a) surface roughness exhibits periodicity, (b) the surface is scratched or bumped with rough patches, and (c) surface heterogeneities are present. The study quantitatively demonstrates the emergence of stick-slip behavior in these scenarios allowing us to verify the thesis of Hocking [3] and Jansons [4]. Our findings serve as a prerequisite for full pore-scale Direct Numerical Simulation (DNS), ensuring a high-fidelity representation of dynamic wetting phenomena in porous media.

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