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Lattice Boltzmann simulations of contact angle hysteresis on chemically square patterned surfaces of large wettability contrast

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ABSTRACT

The contact angle hysteresis on flat and chemically patterned surfaces with large wettability contrast of 86° is studied numerically using an in-house lattice Boltzmann (LB) code. The two-dimensional phase-field-based multiple relaxation time LB model of Liang et al.¹ has been extended to three dimensions. The D3Q19 model is used for both the Cahn-Hilliard equation and the Navier-Stokes equations. The wetting properties of the wall are specified using the contact angle geometric scheme of Ding and Spelt² while the approach of Iliev et al.³ is used to estimate the contact angle.

The code has first been validated by successfully simulating a 3D droplet resting on a chemically homogeneous surface for both acute and obtuse equilibrium contact angles. Then, contact angle hysteresis on chemically patterned surfaces has been investigated. To that end, the intrusion (resp. extrusion) of a liquid phase into (resp. from) a channel has been simulated. The channel is formed by two similarly patterned walls. The pattern consists of non-wetted squares regularly distributed on a wetted surface. The intruding fluid is compelled to move quasi-statically by a body force.

Simulations have been computed with different values of the square size and inter-square distance and their influence on the advancing and receding contact angles has been studied. By rotating the square around its centre the influence of its orientation on the hysteresis has also been investigated. The numerical results proved to be in good agreement with Raj's model⁴. A key parameter to estimate the contact angle hysteresis for such patterned surfaces independently of the square positioning has been identified.

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