The Effect of Surface roughness on the Equilibrium Contact Angle in a Mixed-Wet Medium

Shahab Ghasemi[1], Mohammad Reza Rasaei[1], Sahar Bakhshian[2]

[1]Institute of Petroleum Engineering, School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran
[2]Bureau of Economic Geology, Jackson School of Geosciences, The University of Texas at Austin, Austin, TX, USA

Surface characteristics are important at the micro- and nano-scale level. Surface roughness is one of the main factors influencing the contact angle, as it increases the solid-fluid interfacial area and leads to the droplet impingement on sharp edges of a rough surface. In addition to the surface roughness, anisotropic wetting of chemically heterogeneous surfaces can be a driver to control the contact angle and hence the wetting behavior of a solid surface. In this study, the free energy lattice Boltzmann simulation is applied to investigate the effect of surface roughness and wettability heterogeneity on the equilibrium contact angle in pillar-like pattern surfaces. The rough surfaces are modeled with different pillar shapes and wettability ranging from hydrophilic to neutral wetting conditions. It is found that rectangular pillars lead to the contact line pinning, whereas frustum shapes facilitate the droplet movement.
Furthermore, the effect of relative surface roughness, roughness distribution, and the gravitational force on the equilibrium contact angle was studied. The length scale of the surface patterns is close to the droplet size, for which the Cassie-Baxter and Wenzel equations are not applicable. According to the results, the ratio of the roughness magnitude to the surface area of the droplet is a key factor influencing the equilibrium contact angle. Moreover, droplets on rough surfaces do not necessarily form with the absolute minimum energy. Since a droplet tends to pin on the edge of a pillar, a super-hydrophilic surface behaves as a hydrophobic one.

Keywords: Lattice Boltzmann Method; Surface Roughness; Anisotropic Wetting; Pore-Scale Simulation.