

Simulation of sessile and transient droplets and complex flow dynamics on rough hydrophobic and hydrophilic surfaces using a parallelized Smoothed Particle Hydrodynamics model

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Flow in unsaturated fractures still remains a challenging aspect of vadose zone research. Fracture may create highly efficient preferential flow paths, which trigger the formation of highly complex and non-linear flow modes, such as droplets, rivulets and films. The understanding of these flow types requires adequate numerical techniques. Here we employ a pairwise-force Smoothed Particle Hydrodynamics (PF-SPH) model to simulate sessile and transient droplets as well as flow mode distributions on rough hydrophobic and hydrophilic surfaces. The wettability of solid surfaces depends on their geometrical structure, i.e. the roughness, as well as the fluid properties. Droplets on rough surfaces may exist in a Cassie, Wenzel or Cassie-Wenzel state. Cassie droplets touch the surface only at few points and stay on the top of the rough surface, Wenzel droplets “fill” the surface roughness, and Cassie-Wenzel droplets partially penetrate small surface depressions and/or partially touch only elevated points of the surface.

We employ four types of rough surfaces: (1) with a shape of a sinusoidal function along one direction; (2) with a shape of a sinusoidal function in both horizontal directions; (3) with longitudinal rectangular grooves placed on top of a flat surface and (4) with rectangular bars placed on top of a flat surface. It is demonstrated that the static contact angles of Cassie and Wenzel droplets on rough surfaces is greater than the static contact angle on a smooth surface with the same chemical composition, however, Wenzel droplets exhibit a much stronger dependence on the surface geometry.

Furthermore, we study the impact of the roughness orientation (i.e. an anisotropic roughness) and surface inclination on droplet flow velocities. Simulations show that the droplet flow velocities are lower if the surface roughness is oriented perpendicular to the direction of flow. If the predominant elements of surface roughness are in alignment with the flow direction, the flow velocities increase as compared to smooth surfaces, which can be attributed to the decrease in fluid-solid contact area similar to the classical Lotus-effect. We demonstrate that linear scaling relationships between Bond and Capillary number for droplet flow on flat surfaces also hold for flow on rough surfaces.

To investigate flow mode distribution on rough fracture surfaces we construct surfaces with a self-affine fractal geometry and roughness characterized by the Hurst exponent ζ . We simulate a continuous water flux on the top of the fracture surface. In order to map preferential flow paths, we calculate a cumulative velocity density of the fluid velocity projected onto the solid surface. Areas with high cumulative velocity density, where we define a specific cutoff, can be considered preferential flow paths. The distribution of flow modes, and therefore preferential flow paths on rough surfaces is strongly non-uniform and depends on surface geometry and wetting conditions.