



Three-dimensional smoothed particle hydrodynamics modeling of preferential flow dynamics at fracture intersections on a high-performance computing platform

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The physical mechanisms that govern preferential flow dynamics in unsaturated fractured rock formations are complex and not well understood. Fracture intersections are critical relay points along preferential flow paths and control the partitioning behavior, leading to temporal delay and intermittent flow. In this work, a three-dimensional Pairwise-Force Smoothed Particle Hydrodynamics (PF-SPH) model is being applied in order to simulate gravity-driven droplet flow at synthetic fracture intersections. SPH, as a mesh-less Lagrangian method, is particularly suitable for modeling deformable interfaces, such as three-phase contact dynamics of droplets. The static and dynamic contact angle can be recognized as the most important parameter of gravity-driven free-surface flow. In SPH, surface tension and adhesion naturally emerges from the implemented pairwise fluid-fluid (s_{ff}) and solid-fluid (s_{sf}) interaction force. The model was calibrated to a contact angle of 65° , which corresponds to the wetting properties of water on Poly(methyl methacrylate). The accuracy of the SPH simulations were validated against an analytical solution of Poiseuille flow between two parallel plates and against laboratory experiments. Using the SPH model, the complex flow mode transitions from droplet to rivulet flow of an experimental study were reproduced. Additionally, laboratory dimensionless scaling experiments of water droplets were successfully replicated in SPH. Finally, SPH simulations were used to investigate the partitioning dynamics of single droplets into synthetic horizontal fractures with various apertures ($\Delta d_f = 0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0$ mm) and offsets ($\Delta d_{off} = 1.5, 1.0, 0.5, 0, 1.0, 2.0, 3.0$ mm). The perfect conditions of ideally smooth surfaces and the SPH inherent advantage of particle tracking allow the recognition of small scale partitioning mechanisms and its importance for bulk flow behavior. The aim of this study is to derive an analytical correlation and interpretation of partitioning dynamics, droplet height and aperture.