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Comparison of the Cahn-Hilliard-Navier-Stokes and Molecular Dynamics Approaches for the Simulation of Droplet Coalescence and Wetting Phenomena URBAIN VAES, Department of Mathematics, Imperial College London, BENJAMIN AYMARD, SRIKANTH RAVIPATI, PETR YATSYSHIN, Complex Multiscale Systems Group, Department of Chemical Engineering, Imperial College London, AMPARO GALINDO, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, SERAFIM KALLIADASIS, Complex Multiscale Systems Group, Department of Chemical Engineering, Imperial College London — Diffuse-interface/Cahn-Hilliard equations, coupled to Navier-Stokes (CHNS), have been used extensively over the last few years in fluid dynamics including interfacial phenomena in multiphase systems. Applications range from turbulent two-phase flows to rheological systems and microfluidic devices. But despite the considerable attention CHNS have received, little work has been undertaken to investigate the extent to which they agree with "first-principles" physical models such as those provided by molecular dynamics (MD). Here we compare MD simulations with solutions of the CHNS system obtained numerically using an efficient and systematic finite-element methodology we have developed recently. For this purpose, we consider two paradigmatic model systems: droplet coalescence and droplet motion on a substrate with varying wettability.

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