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Contact line motion from molecular dynamics, the diffuse interface model and the sharp interface model. U. LACIS, FLOW Center, KTH, P. JOHANSSON, Physics & SeRC, KTH, T. FULLANA, S. ZALESKI, d'Alembert, Sorbonne Université & CNRS, S. BAGHERI, FLOW Center, KTH, B. HESS, Physics & SeRC, KTH, G. AMBERG, FLOW Center, KTH — In the context of the sharp interface model Huh and Scriven wrote not even Herakles could sink a solid if the physical model were entirely valid. The resolution of this paradox has occupied a large number of investigators, however a popular fix is to assume a Navier boundary condition for the tangential fluid velocity on the solid surface, which introduces a slip length λ. Nevertheless realistic molecular models show no slip of the first water layer on the SiO2 substrate. Alternate models of the contact line motion involve a dissipative relaxation of the order parameter at the boundary. This relaxation towards contact angle equilibrium involves a contact line friction μ_f. We thus compare interface shapes obtained from a phase-field diffusive-interface model with the results of molecular dynamics (MD) simulation using the GROMACS code. The setup is a simple Couette flow between two plates, with a vapor droplet sheared in the middle of the domain. Another com parison is performed between MD and the sharp-interface model with a slip length and a Generalized Navier Boundary Condition. The sharp interface model is implemented using a VOF method. The role of diffusion across the interface, which is possible in the diffuse interface model, is given particular attention.

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