Abstract Submitted
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Motion of contact line and reconfiguration of two-phase interface: realistic molecular dynamics simulations and Cahn-Hilliard phase field simulations.[1] UGIS LACIS, MICHELE PELLEGRINO, BERK HESS, KTH Royal Inst of Tech, GUSTAV AMBERG, KTH Royal Inst of Tech; Sodert Uni, STEPHANE ZALESKI, Sorbonne Univ and CNRS, SHERVIN BAGHERI, KTH Royal Inst of Tech — Two-phase flow is ubiquitous in both nature and engineering. One example is imbibition of a liquid in a porous material, involving many moving contact lines and reconfiguring two-phase interfaces. These processes are inherently molecular and it is still unclear how to quantitatively model these effects in continuum flow models. To a large extent, this ambiguousness stems from lack of reference data with sufficient accuracy for a wide range of parameters on a simple canonical problem. We choose a two-dimensional Couette problem of droplet between two moving plates and use atomistic molecular dynamics (MD) simulations to create reference data for different plate velocities. We capture steady moving contact line, as well as reconfiguration (splitting) of the two-phase interface, when plate velocity is larger than a critical value. We benchmark the Cahn-Hilliard phase field model against the MD results and provide the parameters for the best representation of the MD reality. Furthermore, we provide insights into key mechanisms responsible for the motion of the contact line as well as for splitting of the two-phase interface. These results will serve as a stepping stone towards developing accurate continuum modelling of many practical problems, such as imbibition in porous media.

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