Finite Element Phase Field Simulation of Dynamic Surface Wetting with Droplets

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ABSTRACT

Wettability plays an important role in the production as well as the application of machine components and can be investigated using molecular dynamic (MD) simulations [1]. The presented phase field model is motivated by the fact that those MD simulations are limited to microscopic length scales as MD simulations go hand in hand with high numerical costs. The model is linked to the MD simulations by its input parameters but larger scales can be considered in numerical simulations.

Based upon the local density (gas/liquid) which serves as the order parameter of the phase field model, and according to an equation of state that corresponds to the MD simulations, the free energy of the system is formulated. Specific contact angles can be regarded by including the surface tensions, between a possibly structured solid surface and the gas and liquid phases, respectively, into the free energy [2]. A global Lagrange multiplier allows to define the average density (liquid volume) of the domain. The FE discretization of this free energy is minimized using an Allen-Cahn evolution equation to find equilibrium droplet shapes and wetting conditions. The fact that the Allen-Cahn evolution equation does not conserve the liquid volume is inconsequential due to the volume constraint.

In order to be able to simulate dynamic wetting scenarios a velocity-density formulation of the Navier-Stokes equations is used to determine the current flow in the liquid as well as in the gas phase. Since the droplet shape and the velocity field need to interact which each other, a coupling between the order parameter of the phase field and the fluid and gas velocities is necessary. This can be achieved by an order parameter convection and the consideration of the surface tension between the gas and the liquid phase within the momentum equation [3].

Details of the algorithmic implementation are discussed and illustrative examples demonstrate the pertinency of the approach.

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