

# ATOMISTIC SIMULATION OF A WETTING/DE-WETTING FLOW

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Standard hydrodynamic models with a no-slip wall boundary condition and zero mass flux phase boundaries become unphysical where a liquid-vapor phase boundary moves across a solid surface. The interface moves, but the fluid on the solid can not if the no-slip condition is enforced. This leads to a flow which is permitted kinematically but has a stress singularity for standard constitutive relationships [1]. To avoid this, slip boundary conditions and a mass fluxes through the interface [2, 3, 4] have both been proposed. Both can relieve the stress singularity. Evaporation and condensation mass fluxes have been modeled with phase-field equations that couple the flow to a chemical potential [2, 3, 4].

We present new observations of the flow in the vicinity of the wetting and de-wetting triple lines of a small liquid roll (a drop that is two-dimensional in the mean) moving on an atomically smooth solid substrate in equilibrium with its own vapor. This flow is studied by simulating the trajectories of atoms that interact via the Lennard-Jones pair potential.

We find that for this case of a liquid drop in equilibrium with its own vapor that evaporation and condensation are substantial components of the flow and at wetting appear to act as anticipated in phase-field models of moving contact line flows [4, 2]. The evaporative flux above the advancing contact line will in part relieve the stress singularity at the wetting contact line, though we also observe some slip in the gas phase. We do not observe as significant a slip at the de-wetting contact line, even at lower temperatures when the liquid and gas phases are made less ‘miscible’. Instead, there is a substantial evaporative flux at this common line, that might resemble phase-field simulation results reported briefly by Jacqmin [2] using a model that incorporates nonlinearity.

## References

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