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Inclusion of fluid-solid interaction in Volume of Fluid to simulate spreading and dewetting for large contact angles[1] KYLE MAHADY, SHAHRIAR AFKHAMI, LOU KONDIC, New Jersey Institute of Technology — The van der Waals (vdW) interaction between molecules is of fundamental importance in determining the behavior of three phase systems in fluid mechanics. This interaction gives rise to interfacial energies, and thus the contact angle for a droplet on a solid surface, and additionally leads to instability of very thin liquid films. We develop a hybrid method for including a Lennard-Jones type vdW interaction in a finite volume, Volume of Fluid (VoF) based solver for the full two-phase Navier-Stokes equations. This method includes the full interaction between each fluid phase and the solid substrate via a finite-volume approximation of the vdW body force. Our work is distinguished from conventional VoF based implementations in that the contact angle arises from simulation of the underlying physics, as well as successfully treating vdW induced film rupture. At the same time, it avoids the simplifications of calculations based on disjoining-pressure, where the vdW interaction is included as a pressure jump across the interface which is derived under the assumption of a flat film. This is especially relevant in the simulation of nanoscale film ruptures involving large contact angles, which have been studied recently in the context of bottom-up nanoparticle fabrication.

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