

Abstract Submitted
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Diffuse-interface modeling of liquid-vapor coexistence in equilibrium drops using smoothed particle hydrodynamics¹ JAIME KLAPP, Cinvestav-Abacus, LEONARDO DI G SIGALOTTI, UAM-A, JORGE TRONCONIS, ELOY SIRA, FRANKLIN PENA, IVIC-Venezuela, ININ-IVIC TEAM, CINVESTAV-UAM-A TEAM — We study numerically liquid-vapor phase separation in two-dimensional, nonisothermal, van der Waals (vdW) liquid drops using the method of Smoothed Particle Hydrodynamics (SPH). In contrast to previous SPH simulations of drop formation, our approach is fully adaptive and follows the diffuse interface model for a single-component fluid, where a reversible, capillary (Korteweg) force is added to the equations of motion to model the rapid but smooth transition of physical quantities through the interface separating the bulk phases. Surface tension arises naturally from the cohesive part of the vdW equation of state and the capillary forces. The drop models all start from a square-shaped liquid and spinodal decomposition is investigated for a range of initial densities and temperatures. The simulations predict the formation of stable, subcritical liquid drops with a vapor atmosphere, with the densities and temperatures of coexisting liquid and vapor in the vdW phase diagram closely matching the binodal curve. We find that the values of surface tension, as determined from the Young-Laplace equation, are in good agreement with the results of independent numerical simulations and experimental data. The models also predict the increase of the vapor pressure with temperature and the fitting to the numerical data reproduces very well the Clausius-Clapeyron relation, thus allowing for the calculation of the vaporization pressure for this vdW fluid.

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