124e Secondary Cohesion and Chemical Potential Models for Diffuse Interfaces

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A recent paper [L. C. Nitsche, A. Nguyen and G. Evans, Chem. Phys. Lett., 397, 417-421 (2004).] developed a cohesive chemical potential (referred to here as "primary" cohesion) for treating liquid-liquid interfaces, which yielded the correct free-surface evolution of drops while seeming to circumvent the characteristic properties of interfacial tension. Diffusion of miscible interfaces was interpreted as a consequence of the same driving force, acting through a different propagator. In this work we refine the chemical potential formulation by semi-analytically subtracting out, at each point within a drop, the corresponding potential for a flat interface at the same distance. The new "secondary" cohesive potential is shown to be consistent with the usual interfacial stress-jump boundary condition, while allowing interfacial "information" to be spread over a significant volume of the drop(s). In other words, the numerically defined interfacial layer need not be "thin". Reduction of parasytic currents in computer simulations is considered. Secondary cohesion is contrasted with (i) two prevailing volumetric versions of interfacial tension, as used in volume-of-fluid and front-tracking numerics, and (ii) the diffuse interface method [D. M. Anderson, G. B. McFadden & A. A. Wheeler, Ann. Rev. Fluid Mech., 30, 139-165 (1998)]. Morphological energy penalties and representations of diffusion associated with the various interfacial chemical potentials are compared. In particular, the double-well mixing energy density of the diffuse interface model can be simplified for certain modeling purposes. Numerical simulations based upon swarms of fuzzy Stokeslets are compared with experiments involving trailing drops and surfaces.