Abstract Submitted
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Coupling Molecular Dynamics to Continuum Computational Fluid Dynamics to simulate Superspreading at the macro-scale[1] EDWARD SMITH, PANAGIOTIS THEODORAKIS, ERICH MULLER, RICHARD CRASTER, OMAR MATAR, Imperial College London — Superspreading surfactants are widely researched, due to their fascinating properties and their many potential applications. However, the mechanism behind superspreading is still poorly understood. Karapetsas et al. (JFM, 2011) demonstrated that surfactant absorption at the contact line is of critical importance by a simple constitutive law in a continuum solver. Molecular dynamics (MD) has the ability to elucidate the details of this mechanism, replacing the constitutive law with explicit modelling of the surfactant, fluid and solid interactions at the contact line. However, MD is computationally-expensive and usually limited to nano-scale problems. We couple both continuum and molecular models in a single simulation so that the mechanism at the contact-line can be explicitly simulated at the molecular scale, while the continuum model can be employed throughout the remaining domain. This allows simulations on scales which approach macroscale experiments while maintaining the vital molecular details. Here, the required coupling techniques to implement the proposed solution are discussed: obtaining continuum boundary conditions by averaging molecules, applying constraint force to the molecular region, addition or removal of molecules and software for coupled simulation on HPC.

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