

Abstract Submitted
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Multiscale approach to studying super-spreading: molecular dynamics and continuum-level models¹ PANAYIOTIS THEODORAKIS, ERICH MULLER, RICHARD CRASTER, OMAR MATAR, Imperial College London — We study surfactant-assisted spreading of fluid droplets on solid substrates. The “super-spreading” problem is a prime example of complex behavior exhibited by such systems, which is not fully-understood. Continuum-level models disregard molecular architecture effects or the specific interactions between the building blocks of the system; hence, they are unable to provide a physical reasoning for the super-spreading mechanism at the molecular level. Molecular dynamics (MD) simulations are restricted to small systems, and are, therefore, unable to provide a continuum description of spreading. Hence we employ a multi-scale modeling approach to study the problem. We use the Statistical Associating Fluid Theory to estimate the intermolecular potentials between the solvent and the surfactant particles using a top-down coarse-grained approach. As a result, we have achieved quantitative matching of our simulations to experimental macroscopic thermophysical properties. Based on these interactions, we perform MD simulations by taking into account, the molecular architecture of surfactants, and we estimate the relevant microscopic parameters and boundary conditions for use in our continuum description. Results from our multiscale approach will be presented at the meeting.

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Omar Matar
Imperial College London

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