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(G*) (POS-26) Towards a Unifying Model for Droplet Spreading Using an Exponential Law: A Molecular Dynamics Study

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Over the recent decades, molecular dynamics (MD) has emerged as a promising tool for investigating droplet interaction with surfaces and its local effects. We examine the classic problem of spreading liquid droplets on surfaces that govern myriad processes ranging from coating and printing to even biological systems. Spreading is usually studied using only the evolution of contact radius r with respect to time. In the complete wetting regime, the droplet fully spreads on the surface, whereas in partial wetting, it assumes a cap-shaped form signified by a contact angle. A simple power law of the form $r \propto t^{\alpha}$ can describe spreading in the complete wetting regime.[1] However, empirical parameters are often proposed to model its behavior if the droplet does not completely spread on the surface. Additionally, neither case has established a universal exponent α. In this study, we use MD simulations of water droplets spreading on a Lennard-Jones surface with various degrees of wettability to investigate a new spreading model. A new method describing the contact radius of droplets in MD simulations is proposed and verified via comparison with established techniques. The applicability of the non-dimensional form of the model to both wetting regimes is explored. Furthermore, the equidimensional equation $\frac{t}{r}\frac{dr}{dt}$ is also discussed following the work of Stone *et al.*[2] The dimensionless form reveals the effect of surface wettability and its contact angle on the exponent α. The results from our unifying approach to the study of spreading lead to a deeper understanding of the process, particularly in the partial wetting regime.

[1] Nieminen, J. A.; Abraham, D. B.; Karttunen, M.; Kaski, K. Molecular Dynamics of a Microscopic Droplet on Solid Surface. Phys. Rev. Lett. 1992, 69, 124–127.

[2] Bird, J. C.; Mandre, S.; and Stone, H. A. Short-time Dynamics of Partial Wetting. Phys. Rev. Lett. 2008, 23, 234501.

Keyword-1

Droplet Spreading Law

Keyword-2

Partial Wetting

Keyword-3

Complete Wetting

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