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Dynamical insights into the mechanism of a droplet detachment from a fiber†

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Quantifying the detachment behavior of a droplet from a fiber is important in many applications such as fog harvesting, oil–water separation, or water management in fuel cells. When the droplets are forcibly removed from hydrophilic fibers, the ease of detachment strongly depends on droplet volume and the rate of the process controlled by the applied force. Experiments, conducted on a ferrofluid under magnetic force, as well as continuum level calculations from fluid mechanics have so far been unable to resolve the time-dependent dynamics of droplet detachment and, most importantly, to assess the role of the applied force as the key determinant of the volume of the droplet residue remaining on the fiber after detachment. In the present work, we study the mechanism of water droplet detachment and retention of residual water on smooth hydrophilic fibers using nonequilibrium molecular dynamics simulations. We investigate how the applied force affects the breakup of a droplet and how the minimal detaching force per unit mass decreases with droplet size. We extract scaling relations that allow extrapolation of our findings to larger length scales that are not directly accessible by molecular models. We find that the volume of the residue on a fiber varies nonmonotonically with the detaching force, reaching the maximal size at an intermediate force and associated detachment time. The strength of this force decreases with the size of the drop, while the maximal residue increases with the droplet volume, V, sub-linearly, in proportion to the $V^{2/3}$.

1 Introduction

The adherence to, and removal of droplets from cylindrical fibers underlie applications from fog harvesting,[1–4] oil–water and oil–air separation,[5–8] and water transport in fuel cells.[9,10] In all these applications, the performance of the system depends on the conditions for the liquid release from, and the extent of retention by the fibers,[11] and quantitative information about droplet–fiber interaction is of great value in designing a new product. The equilibrium shape of a droplet on fiber[12–15] has been examined in reasonable depth in the literature.[16,17] For droplets and fibers in the micrometer range, it is known that when the gravity effect is negligible, two topologically distinct droplet shapes occur: asymmetric clamshell and axially symmetric barrel conformations, depending on the droplet volume, the contact angle, and the fiber radius.[17] Fiber roughness and fiber orientation can also have a significant effect on the equilibrium shape of droplet and wettability.[18–20]

Motivated by various applications in the field of automotive engineering, *e.g.*, removal of airborne oil droplets from the engine exhaust *via* the so-called coalescence filters, experimental studies have been conducted to measure the force required to detach a droplet from a fiber and to use that information to estimate an allowable velocity for the flow of smoke through a filter.[21–24]

Using continuum simulations, the equilibrium shape of an isolated droplet deposited on a fiber under the influence of an enhanced external body force has been determined recently by Ameri *et al.*[25] These authors incrementally raised the magnitude of the external body force applied to a droplet until no equilibrium shape/position could be obtained for the droplet on the fiber. They referred to the maximal force the droplet could sustain in an equilibrated state as the force of detachment and studied its dependence on fiber diameter, fiber roughness, fiber wettability, and droplet volume.[18] The continuum simulations,[25] however, could not resolve the time-dependent dynamics of droplet detachment, and more importantly, the volume of the droplet residue on the fiber. The latter is especially important from an industrial viewpoint as it affects the repeatability of the droplet separation processes. For instance, to increase the efficiency of fiber filters, the volume of the residue should be suppressed to prevent the clogging of the fiber network,[20,26,27] while in water harvesting increasing the residue volume on the fiber arrays improves the net's efficiency.[2] The residual volume depends on the droplet volume, the contact angle, fiber radius,

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