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Influence of Contact Angle Dynamics on Interaction between Mist Droplets and Isolated Cylindrical Fibres

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Abstract

Separation of liquid droplets or mist that are generated in anthropogenic or industrial processes is typically accomplished through coalescence filtration, employing highly porous fibrous media. One of the critical factors affecting the efficiency of mist filtration, besides filter or pore structure, packing density, permeability, etc., is wettability of mist on the filter surface. While the filtration efficiency at low particle concentrations is explained well by single fibre filtration theory, there is yet no comprehensive model for accounting the possibility of an initially captured mist droplet getting re-entrained into the flow due to the kinetic interactions with the fibre surface. In the present study, computational simulations are carried out to investigate the effect of contact angle hysteresis and dynamic contact angles (encapsulating super-oleophilic and super-oleophobic) on the dynamics of a mist droplet interacting with a single fibre. For each wetting condition, two fibre diameters d_f = 0.5 and 1 μm, and two droplet impact locations on the fibre (corresponding to an offset from centre of H = -2 and 0.25) are considered, and the flow velocity is kept constant at u_o = 1 m/s. The simulations are carried out using the Volume Of Fluid (VOF) interface capturing approach in the finite volume solver interFoam available within OpenFOAM. It is found from the present simulations that for a given equilibrium contact angle, an increase in contact angle hysteresis, limits droplet-spreading on the fibre to the extent that for some cases the droplet pinches off the fibre with or without a fraction of the droplet retained/ captured. It is also seen that an increase in contact angle lowers the potential for mist capture for (H = 0.25) and a significant reduction in the equilibrium wetted area for (H = -2).

Introduction

Removal of liquid aerosols is of significant importance in a variety of industrial and automotive applications for both, economic and toxicological reasons. The most commonly used technique for mist filtration is by employing highly porous fibrous, knitted or foam media [1]. Mist filtration process is characterized by an initial transience until the captured mist coalesce inside the filter media to form large fluid structures, and an equilibrium state of fluid saturation. While respirators typically operate at low levels of fluid saturation, relatively higher levels typically describe the long term operation of industrial and automobile filters. In any case, the knowledge of the capture efficiency of mist by the filter media is paramount for efficient design and optimization.

Most industrial oil-mist filters are oleophilic in nature due to their advantages in fluid retention, while more recently, carefully engineered oleophobic media are also preferred due to the advantages in reduced pressure-drops resulting from enhanced drainage of captured oil. The effect of oleo-phobicity or -philicity of the filter media on the overall filtration efficiency has received some attention in recent years [2] for conditions of high fluid saturation. However, the capture efficiency of single fibres (or low saturation) is estimated predominantly only by the classical single-fibre theory [3] that is originally based on dust filtration - with the assumption that a particle sticks to the surface of the filter once in contact. This may not necessarily be true for mist filtration applications as the effects of wetting dynamics on the filter surface can potentially result in the droplet sliding on the surface and even leading to re-entrainment into the flow - resulting in a lower capture efficiency than that predicted by single-fibre theory. However, there is yet no comprehensive model characterizing the interactions between mist and the filter surface accounting for the wide possibilities in contact angles and associated hysteresis that can arise from the range of materials (metal/ polymer/ cellulose) used to make filter media.

It is widely accepted that experimental determination of contact angles on micro-fibre filter media is exceedingly difficult due to limitations in the resolutions of current imaging equipment [2] - which limits accurate experimental characterization of wetting on mist filters. Pore-scale or isolated computational fluid dynamics (CFD) simulations of the mist filtration process using advanced droplet- and interface-tracking approaches provide unique advantages in allowing precise definition of contact angles, and other interfacial and fluid properties. In the present study a fundamental analysis is carried out to study the effect of wetting dynamics on the interaction between a single droplet mist and an isolated fibre, by varying the equilibrium and dynamic limiting contact angles to represent super-oleo-philic to -phobic media with low or high contact angle hysteresis.

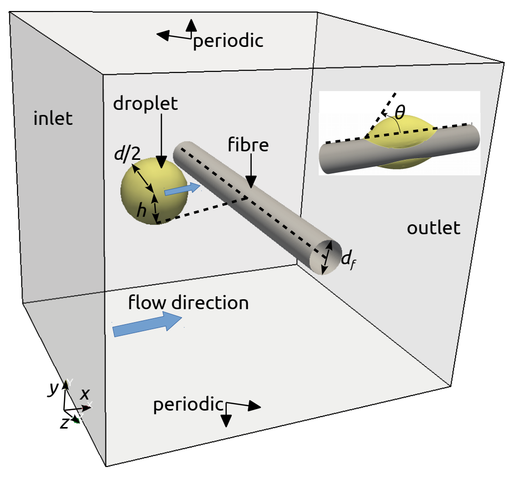


Figure 1: Schematic of the geometry and computational domain

Geometry and Computational Domain

A droplet of Diethylhexyl Sebacate (DEHS) oil mist of diameter d is carried by a steady stream of air at u_o = 1 m/s such that it impacts or intercepts a cylindrical fibre of diameter d_f at a location represented by an eccentricity h, as shown in Fig. 1. The droplet diameter is kept constant in the present study at $d = 2\,\mu$m which is typical of oil mist generated in many applications including lubricated machining [4]. The wetting characteristics of the fibre surface are specified using equilibrium (θ_e), advancing (θ_a) and receding (θ_r) contact angles based on the local velocity of the oil-air interface tangential to the filter surface.

The simulations are carried out on fully structured hexahedral mesh configuration with a uniform velocity at *inlet*, atmospheric pressure at the *outlet* and periodic boundary conditions imposed on the *sides* of the domain (Fig. 1). All simulations are carried out with constant fluid properties: ρ_l = 912 kg/m^3, μ_l = 0.0228 Pa-s, ρ_g = 1.2 kg/m^3, $\mu_l = 1.8^{-5}$ Pa-s and σ = 0.032 N/m; the contact angles (static and dynamic) applied between the oil and filter surface are discussed in the following section.

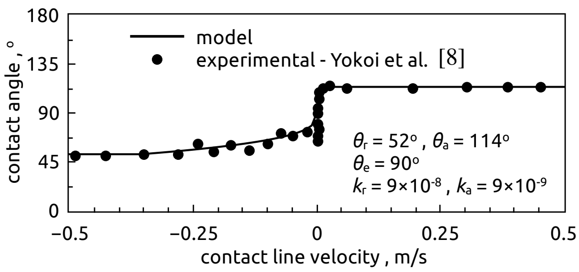
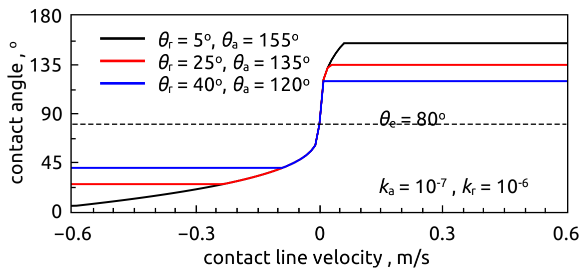
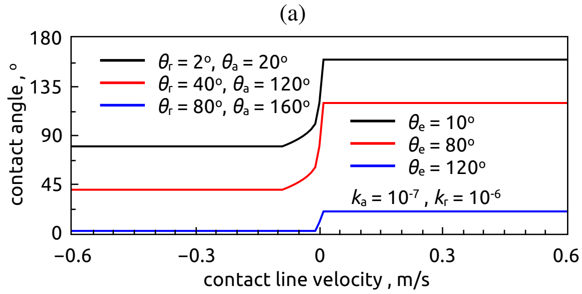


Figure 2: Dynamic contact angle model from Yokoi et al. [8]



(a)



(b)

Figure 3: Dynamic contact angle models used for the study

Methodology

The governing equations for the conservation of mass and momentum are solved iteratively using the transient, finite-volume solver interFoam available within OpenFOAM. The interface between the two fluids (oil and air) is determined by solving for the transport of a volume fraction (α where $\alpha_l + \alpha_g = 1$; the subscripts l or g represent liquid or gas) function where a value of 0 or 1 represents the computational cell occupied by air or oil respectively. The solver uses an algebraic volume-of-fluid (VOF) method which is well established for multiphase flow problems of the type considered for the present study [5, 6]. In the VOF technique, a single set of mass and momentum conservation equations as given below, are used to describe the system where the local fluid properties are determined based on the volume fraction.

Test	Parameters	θ_e	θ_a	θ_r
Hysteresis	$d_f = 0.5\,\mu m$ with $h = 0$ or $1.125\,\mu m$ and $d_f = 1\,\mu m$ with $h = 0$ or $1.25\,\mu m$	80°	0° 40° 25° 5°	0° 120° 135° 155°
Wetting	$d_f = 0.5\,\mu m$ with $h = 0$ or $1.125\,\mu m$ and $d_f = 1\,\mu m$ with $h = 0$ or $1.25\,\mu m$	10° 80° 120°	0, 2° 0, 40° 0, 80°	0, 20° 0, 120° 0, 160°

Table 1: Test conditions considered for the present study

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

$$\partial(\rho\vec{u})/\partial t + \nabla \cdot (\rho\vec{u}\vec{u}) = -\nabla p + \nabla(\mu\nabla\vec{u}) + \rho\vec{g} + f_\sigma \tag{2}$$

$$\partial\alpha_l/\partial t + \nabla \cdot (\alpha_l\vec{u}) + \nabla[\vec{u}_c\alpha_l(1-\alpha_l)] = 0 \tag{3}$$

where $\vec{u}_c$ is the compression velocity, which ensures a sharp representation of the interface and reduced numerical smearing. The interfacial surface tension force density (f_σ) that is incorporated for alleviating any computational issues associated with the discontinuous pressure-jump across the interface [6] is based on the continuum-surface-force model [7] as:

$$f_\sigma = -\sigma[\nabla \cdot (\nabla\alpha_l/|\nabla\alpha_l|)](\nabla\alpha_l) \tag{4}$$

The conservation equations are solved using the combined PISO-SIMPLE algorithm and the Multidimensional Universal Limiter with Explicit Solution (MULES) algorithm is employed for the volume-fraction transport equation [6]. The contact angle on the fibre surface is modeled based on the interface capillary number ($Ca = \mu u_{iw}/\sigma$) following Yokoi et al. [8] as:

$$\theta = \begin{cases} \min[\theta_e + (Ca/k_a), \theta_a] & \text{if } u_{iw} \geq 0 \\ \max[\theta_e + (Ca/k_r), \theta_r] & \text{if } u_{iw} < 0 \end{cases} \tag{5}$$

In Eq. (5), k_a and k_r are empirically determined material parameters for advancing and receding contact angles respectively. An example for determining k_a and k_r is shown in Fig. 2, and further details on the model are available in Yokoi et al. [8].

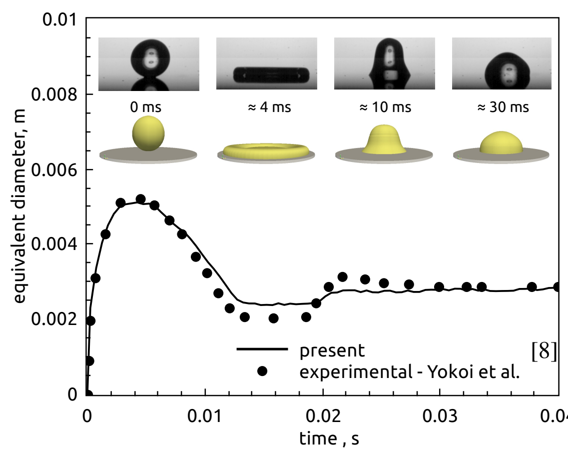
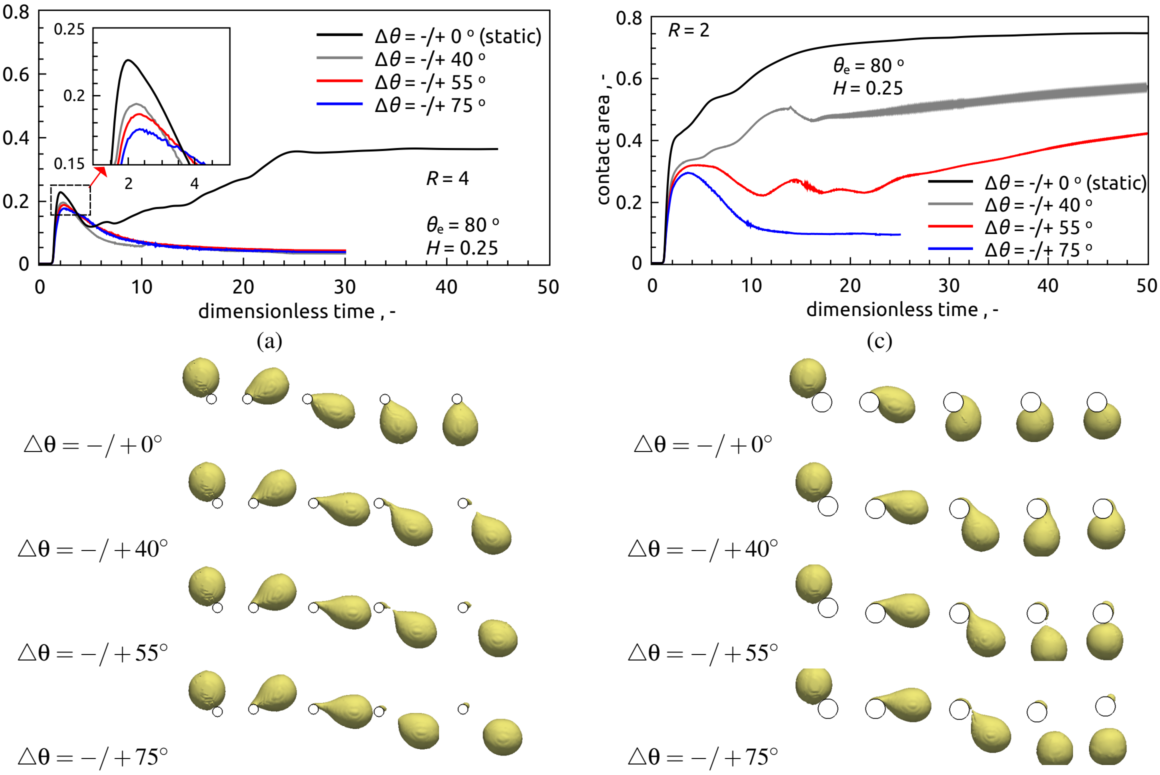


Figure 4: Comparison of predicted (present) equivalent diameter against Yokoi et al. [8]

In the present study, the influence of wetting dynamics is investigated in two parts: (i) influence of contact angle hysteresis for given equilibrium contact angles; (ii) effect of contact angle (each with a specified hysteresis). The dynamic contact angle



(b) τ = 0,1.25,2.5,3.75 and 4.3; flow from left to right

(d) τ = 0,2.4,4.65,6.65 and 11.2; flow from left to right

Figure 5: Influence of contact angle hysteresis on the interaction between an impacting oil mist droplet and fibre

models chosen for the present study are shown in Fig. 3. A summary of the operating parameters and contact angles considered for the present CFD simulations is provided in Table-1.

Validation

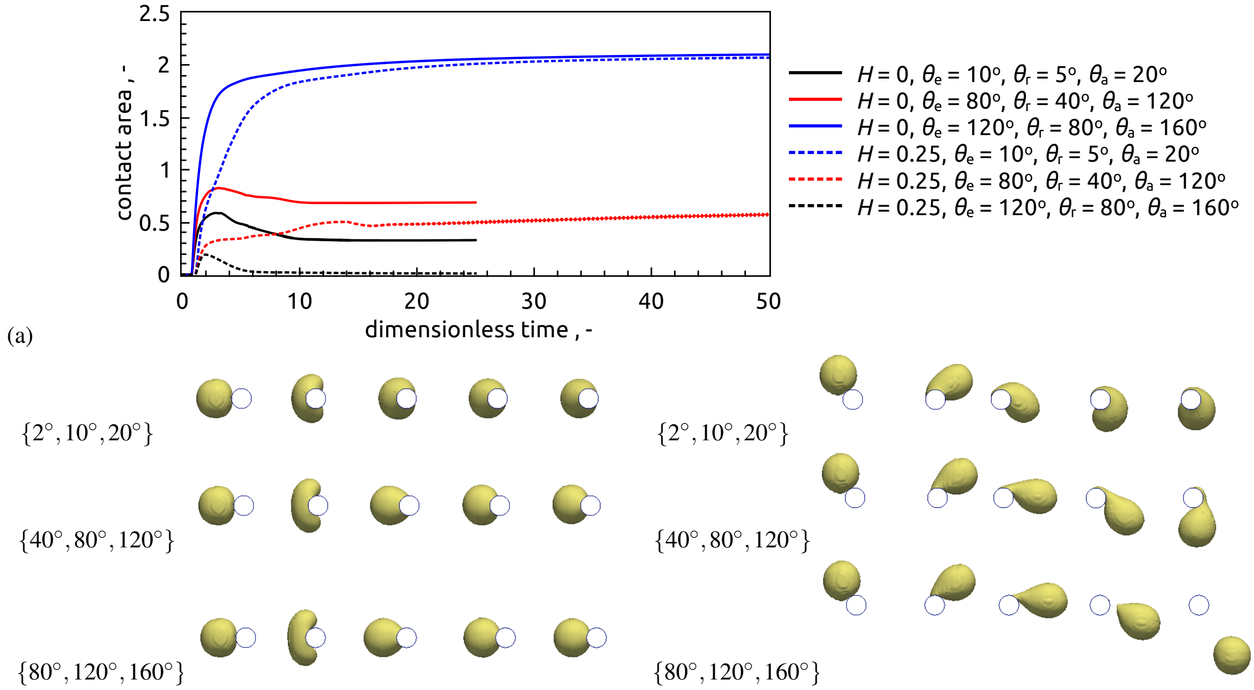
The VOF methodology in interFoam available within OpenFOAM has been widely validated in the literature [5, 6] for problems of the type considered in the present research. The present CFD methodology, particularly the incorporation of the dynamic contact angle model using customized libraries is validated in the present study by evaluating the dynamics of wetting of a droplet impacting a stationary flat surface - a case that was originally used in Yokoi et al. [8] for the development of the dynamic contact angle model. A droplet of water (ρ_l = 1000 kg/m^3, $\mu_l = 10^{-3}$) falls due to the influence of gravity, in an ambiance of air (ρ_g = 1.25 kg/m^3, $\mu_g = 1.82\times10^{-5}$) and impacts a flat surface at a velocity of 1 m/s. The contact angle between water and the surface is the same as that shown in Fig. 2, and the air-water interfacial tension is assumed to be 0.072 N/m.

The comparison of the equivalent diameter (calculated based on wetted surface area) predicted from the present simulations against the experimental data of Yokoi et al. [8] is shown in Fig. 4. Instantaneous shapes of the droplets at different times are also shown in the figure and compared with the experimental/ photographs in Yokoi et al. [8]. It can be seen in the figure that the predictions from the present methodology are in excellent agreement with the literature, thereby validating the incorporated dynamic contact angle model for the study, and reinforcing the validity of the present computational approach.

Results and Discussion

The influence of contact angle hysteresis is studied by employing four different limiting values of advancing and limiting contact angles as shown in Fig. 3(a) for conditions described in Table-1. The nature of droplet interaction (capture or detachment) on the fibre is quantified in terms of the wetted area for any given set of operating conditions, and qualitatively characterized from visual representation of the results from CFD. The latter is important as any given contact area can represent high contact angles, or lower mass of liquid retained on the surface. Figure 5 shows the transience of dimensionless contact area (ratio of wetted area to $\pi d^2/4$) for eight different representative cases. In the figure, the dimensionless time, diameter ratio and eccentricity are defined as $\tau = tu_a/d$, $R = d/d_f$ and $H = (h-0.5\times d)/d_f$ respectively, and $\triangle\theta = \theta_a - \theta_e = \theta_e - \theta_r$. It is seen from the figures that an increase in contact angle hysteresis results in decreased spreading of the droplet on the fibre surface. This is because, for a given droplet kinetic energy, both, an increase in advancing contact angle and decrease in receding contact angle results in the stretching of the oil-liquid interface close to the surface and causes an reduction in contact line velocity. This is evident from Figs. 5(a,c) where the initial ($\tau < 10$) dimensionless contact area is consistently lower for relatively greater values of $\triangle\theta$. Although the $\triangle\theta = 75°$ can imply super-oleophilic contact angles on parts of the contact line, it is seen that when associated with a large advancing contact angle, this can lead to droplet detachment post-capture (partial or full) - implying that large hysteresis can be significantly detrimental to mist filtration due to potentially lower capture efficiencies. For a lower eccentricity (H = 0; data omitted for brevity) it was found that an increase in hysteresis reduced the steady (equilibrium) wetted area on the fibre. Literature [9] suggests that this can potentially lead to droplet re-entrainment as the effective force (drag) required for droplet detachment is relatively lower.

The influence of wettability is studied by employing three different equilibrium contact angles (each with an associated hysteresis) as shown in Fig. 3(b) for conditions described in Table-1. Figure 6 shows the transience of dimensionless contact area for six different representative cases. It is seen that an increase



(b) $\tau = 0, 1.25, 2.5, 4, 6.9$; flow from left to right (c) $\tau = 0, 1.15, 3.65, 6.65, 11.15$; flow from left to right

Figure 6: Influence of contact angle on the interaction between an impacting oil mist droplet and fibre; the angles represent $\{\theta_r, \theta_e, \theta_a\}$

in θ_e consistently deteriorates that capture potential of the filter surface, particularly for higher value of eccentricity. For H = 0, it is seen from the figure that the final or steady state contact area is significantly lower for greater contact angles. It is also interesting (see Fig. 6(a)) that for both the eccentricities considered, the final equilibrium wetted area reach an asymptotic value (for fully captured drops) implying a strong influence of surface tension as expected for the micro-droplet/-fibre cases considered. The simulations have revealed that classical single-fibre efficiency theory may be applicable only to a very limited oleophilic media and further research is required to fully characterize the droplet-fibre interactions involved in mist filtration.

Conclusions

Computational simulations are carried out to evaluate the influence of contact angle hysteresis and wettability on the dynamics of droplet-fibre interactions relevant to mist filtration applications. The key findings from the present research are follows:

- Application of classical single fibre theory may become invalid in predicting capture efficiencies for high contact angles, or fluid-fibre combinations with high θ-hysteresis.
- Increase in hysteresis lowers the contact area between the droplet and fibre, and may lead to droplet detachment.
- Increase in contact angle or -phobicity reduces the droplet capture efficiency.

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