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Simulating Plateau-Rayleigh instability and liquid reentrainment in a flow field using a VOF method

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Abstract

Plateau-Rayleigh Instability (PRI) is the well known phenomena of the breakup of a liquid column or cylinder. Such a process is integral to the operation of a range of natural and anthropogenic systems, such as gas-liquid and liquid-liquid separators, fuel cells, the accumulation of dewdrops on spider webs, and many more. Volume Of Fluid (VOF) methods, such as available in OpenFOAM, should be able to accurately resolve PRI in such systems. One such system, in which PRI is integral, is the filtration of oil or water aerosol mists using fibrous filters. In many cases, entrainment (or carryover) of liquid from fibers occurs. The mechanisms behind such entrainment are poorly understood. This work will validate the OpenFOAM VOF against classical PRI theory, both with and without a secondary fluid phase flowing through the system (e.g. air). Furthermore, the work will utilise the validated two-phase VOF solver to examine the phenomena of liquid reentrainment from mist filters.

Introduction

Fine liquid jets and liquid films on cylindrical elements will, under most circumstances, be unstable and break up into a series or array of small droplets via Plateau-Rayleigh instability [7]. There are a number of applications where the simulation of this phenomena may be advantageous, examples include, fiber manufacturing, wire coating, electro-spinning, fuel cells, optic fibers, surgical textiles and mist/droplet filtration.

The convex surfaces of a cylindrical element (such as a fiber) indicate that positive curvatures will exist on any coating films that develop; leading to a positive Laplace excess pressure acting on the film-air surface [6]. The Laplace pressure will generally try to spread a liquid over a surface. In the case of a fiber, where the film radius at the solid-liquid interface is different from that at the liquid-vapor interface, this pressure will act to force the liquid out of the film and in doing so introduce an instability. Here, the liquid surface tension will act to minimize the free surface area, thereby creating the instability [8]. This instability will cause the liquid film to undulate and break up into an array of droplets. This was first observed by Plateau, who demonstrated that all axisymmetric wavelengths greater than the liquid cylinder (film) circumference will be unstable. Of all the possible wavelengths, the fastest mode will predominate [6]. This is the commonly known phenomena, of Plateau-Rayleigh instability and for a thin film on a fiber the predominant wavelength (λ) will be $2\pi\sqrt{2}r_f$ [6], where r_f is the radius of the fiber.

Therefore the thickest possible film which could exist, on a thin cylindrical fiber, would be when the wavelength was equivalent to the circumference of the liquid cylinder coating the fiber. Such that $2\pi\sqrt{2}r_f = 2\pi(r_f + h_t)$. Mullins et al. [4] showed that this imposes a limit on the film thickness, h_t, of $h_t = r_f(\sqrt{2}-1)$.

The accurate resolution of Plateau-Rayleigh instability is vital for realistic 3D simulation of systems such as liquid (mist) filters [1]. In order to develop CFD models for complex droplet-fiber (and fluid flow) systems, such as fibrous filters and Proton Exchange Membrane (PEM) fuel cells, we need to first ensure that the simulations of the micro-scale physico-chemical processes are accurate. Given that coalescing filters work by capturing liquid aerosol droplets and that these droplets (assuming they wet the fibre) spread over the fiber to form a thin film, the accurate simulation of Plateau-Rayleigh instability will be important in any attempt to simulate such droplet-fiber systems as a whole. We seek to demonstrate that such simulations can be accomplished using an open-source Computational Fluid Dynamics (CFD) Volume-Of-Fluid (VOF) solver; thereby demonstrating that CFD is an appropriate, accessible and viable technique for the simulation of droplet fibre systems. The simulation then, does not rely on the derivation of an appropriate numerical expression, but on a more fundamental solution to the momentum and continuity equations.

Methodology

Our simulations utilised the open-source OpenFOAM CFD package (Silicon Graphics Inc. Sunnyvale, USA). An unstructured hexahedral mesh was generated over a single 10 μm diameter cylinder, located centrally and oriented either vertically or horizontally within a square prism, with the longest side being equal to (or in the reentrainment studies greater than) the length of the fiber. A fluid column (film) was placed around the fibre with a specified thickness. The flow field within the film was set to have zero velocity; i.e. it is stationary. A cyclic boundary condition was set between the two faces of the geometry intersected by the fiber. The solver used was a three-dimensional unsteady solver, that utilised the Multidimensional Universal Limiter with Explicit Solutions (MULES) algorithm to handle the transport equation and the Pressure Implicit with Splitting of Operators (PISO) algorithm for the coupled pressure-velocity fields.

The transport models implemented in OpenFOAM allow for the contact angles of the two-phase interface to be defined. This required specification of the parameters θ_0, $\mu\theta$, θ_A and θ_R. The value of θ_0, the static contact angle, was selected based on published experimental data [1]. The value of the dynamic contact angle velocity scale$\mu\theta$ was set to 1. The values of θ_A and θ_R (the limiting advancing and receding contact angles, respectively) were set to 1.047 and 0.01 radians. These values are not the dynamic contact angles of the system, but limiting ranges for the simulation and were chosen to give the system a wide permissible range and also to avoid negative numbers and zeros, which may have caused the calculation to become unstable.

Table 1: Film thicknesses and observed break-up, without flow field. The maximum theoretical h_t is 2.07 μm

h_t (μm)	Break up u=0 m/s / u=0.1 m/s	Notes	t (s) to Break up u=0 m/s / u=0.1 m/s
1	no / no	unstable*	- /-
1.1	no / no	unstable*	- /-
1.2	no / no	unstable*	- / -
1.3	no / no	unstable*	- / -
1.4	yes / yes	stable (2)$^+$	0.00054 / 0.00041
1.5	yes / yes	stable (2)$^+$	0.00055 / 0.00041
1.6	yes / yes	stable (2)$^+$	0.00074 / 0.00062
1.7	yes / yes	stable (2)$^+$	0.00074 / 0.00062
1.8	yes / yes	stable (2)$^+$	0.00102 / 0.00086
1.9	yes / yes	stable (2)$^+$	0.00108 / 0.00086
2	yes / yes	stable (2)$^+$	0.00108 / 0.00087
3	yes / yes	stable (2)$^+$	0.0011 / 0.0009
5	yes / yes	stable (2)$^+$	0.0011 /0.0009

- the film does not break up into droplets, however the surface profile changes over time.

$^+$ - the film breaks up into 2 axisymmetric droplets

In order to test the onset of Plateau-Rayleigh instability, the thickness of the film was varied between simulations. The maximum possible film thickness for a given system can be determined using Equation h_t. Therefore by simulating film thicknesses either side of this maximum value, the effectiveness of OpenFOAM in simulating the Plateau-Rayleigh instability can be determined.

In addition to the "static" cases examined, a laminar (steady) flow solver was used to impose a second fluid (flow) field (air from left-right of geometry) on the original fluid (droplet/film) phase (oil) which allowed droplet motion and displacement in a flow field to be examined, and permitted comparison with previous results [1]. Gravitational forces were not considered in simulations, as it has been proven insignificant for $d_d < 100\mu m$.

Results and Discussion

Simulations were conducted on fiber lengths of 175, 225 and 500 μm to ensure that the (cyclic) geometry boundary did not influence the film break-up. According to The equation for h_t, the thickest film which should exist on a 10 μm diameter fiber is 2.07 μm. Therefore film thicknesses around this value were examined. The results of the simulations run without the presence of a flow field, are given in Table 1. Under-relaxation was also utilized, by placing relaxation factors of 0.8 and 0.3 on the initial estimates of the pressure and velocity respectively.

Fig. 1 shows the break-up of a 2 μm thick film on a 10 μm diameter fiber. Fig. 1a shows the initial film (i.e. at t = 0 s), which simply displays the liquid film on the fiber. Fig. 1b shows the film at t = 0.00078 s, which has begun to undulate and no longer appears completely cylindrical. Fig. 1c, d and e show the fairly rapid formation of axisymmetric droplets at t = 0.000845, 0.00086 and 0.00087 s, respectively. Fig. 1f shows a distinct centrally located axisymmetric droplet at t = 0.00092 s, with droplets immediately above and below extending to the bounds of the geometry.

The results in 1 show that the simulated break up occurs at a lower value of h_t than predicted by h_t. This however is permissible, as the value obtained from h_t represents a maximum allowable film thickness. Therefore it is clear that the solver will not allow a physically unrealistic film to exist on the fiber. The films that do not break-up are considered unstable, as the fluid surface does not attain a consistent conformation, i.e. remains clearly as a film, however the surface position exhibits slight fluctuations over time.

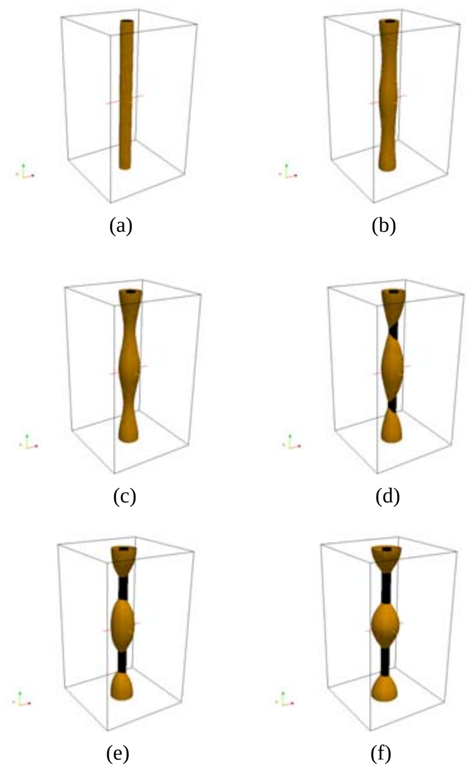


Figure 1: A series of images showing the simulation of the break-up of a liquid film under the influence of Plateau-Rayleigh instability, from t=0 (a) to t=0.00092 (f)

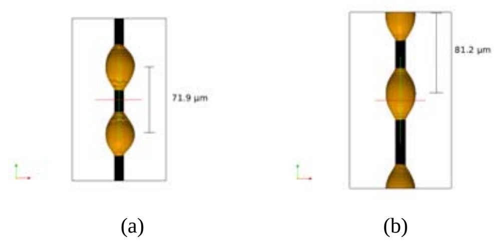


Figure 2: The space between droplets formed by the simulation of the break up of a 2 μm film via the Plateau-Rayleigh instability, in absence of flow, (a), and in the presence of flow, (b)

The film break-up was also simulated in the presence of flow, using the same film thicknesses. When compared with the results in 1, however, it was found that the maximum film thickness that the solver will allow is ultimately no different in the presence of a flow field; however, the break-up of the film does however occur at an earlier time-step in the simulation. So the presence of air flow velocity (u) (0.1 m/s in this case) will influence the time to break up of a liquid film but not the film stability. Additionally, the droplet positioning on the fibre is different in the presence of flow; this can be seen in Fig. 2. This effect was verified over multiple simulations and is likely due to the system acting to minimize overall drag force.

The simulation of the break up of a liquid film into an array of droplets via Plateau-Rayleigh instability could be further validated using experimental observations [6], where droplet spacing was found theoretically to (usually) correspond to the length of the predominating wavelength. This wavelength as determined by Quere [6], is $2\pi\sqrt{2}r_f$, and therefore on a 10 μm diameter fiber, the average droplet spacing will be 44.43 μm. This however, relies on $h_t << r_f$, which is incorrect in our case since we have a 2 μm film on a 5 μm radius fiber. As is shown in Fig. 2 we can measure droplet spacing from our results. Here the droplet spacing can be seen to be greater in the presence of flow, which is likely related to the earlier film break up. Mean droplet spacing for multiple simulations was found to be 71.9 $\pm$ 5 μm for u=0 and 81.2 $\pm$ 5 μm for u=0.1, with no significant difference observed for higher values of u.

The droplet spacing was found to be consistent, regardless of fibre length and is not influenced by the presence (or absence) of cyclic boundary conditions. However, given the difference between the simulated and theoretical droplet spacing on this fibre diameter, it was decided to explore the simulated droplet spacing further. Fig. 3 shows the simulated (VOF) and theoretical (Quere [6] theory) droplet spacing resulting from the break-up of a film of thickness h_t on a number of fibre diameters. It can be seen that good agreement between theory and simulation exists between 15 and 20 μm and near 30 μm. Some deviation occurs above and below these values. This indicates that the break-up of a liquid film into a droplet array can be simulated reasonably well.

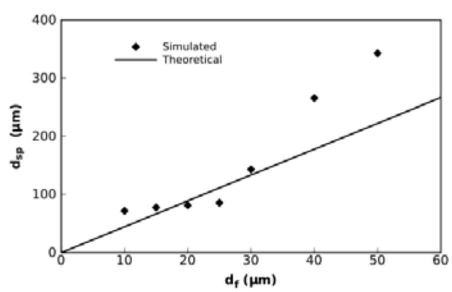


Figure 3: Simulated and theoretical [6] droplet spacing, resulting from the break-up of a liquid film of thickness h_t on different fiber diameters

Mead-Hunter et al. [1] introduced a theoretical model, which described the force required to move a droplet along a fiber. In this model a term describing the displacement (r) of the mass centre of the droplet away from the center of the fiber was provided. Increasing r was found, both theoretically and experimentally, to decrease the force required to move a droplet. This effect should then be present in the simulated system.

Droplet displacement (r) in air flow was examined by varying the flow velocity (u) acting on the system. r=0, when u=0, and increases as u increases.

A droplet that does not drain at u=0.1 m/s, may drain at u=0.2 m/s. This is due to the combined effects of increased air flow force acting on the droplet and the effect of r, which decreases the force needed to drain a droplet of a given size.

At u=0.1 m/s the droplet appears slightly displaced, with a small value of r. At u=0.2 m/s, the value of r is slightly larger and the droplet drains down the fiber much more readily. Hence less force is required in order to initiate droplet motion. The influence of r may be seen in Fig. 5a, where the relationship between u, F and r is shown. Here r is considered in terms of r/b (where b is the droplet radius) as this allows droplets and fiber of different sizes to be compared [5].

The force acting on a droplet in the simulation may be calculated by extracting the gradients from the surface normals at the two-phase interface and multiplying by the liquid viscosity (performed using a custom script). The simulated force can be readily compared to the force predicted by classical drag equations (assuming a spherical droplet). The drag force (F_d) on a sphere is given by; $F_d = 3\pi\rho d_d u$, and the drag on a cylinder (fiber) by; $F_c = \frac{1}{2}\rho u^2 d_c L C_D$, where d_c is the cylinder diameter, L the cylinder length, and C_D the drag coefficient.

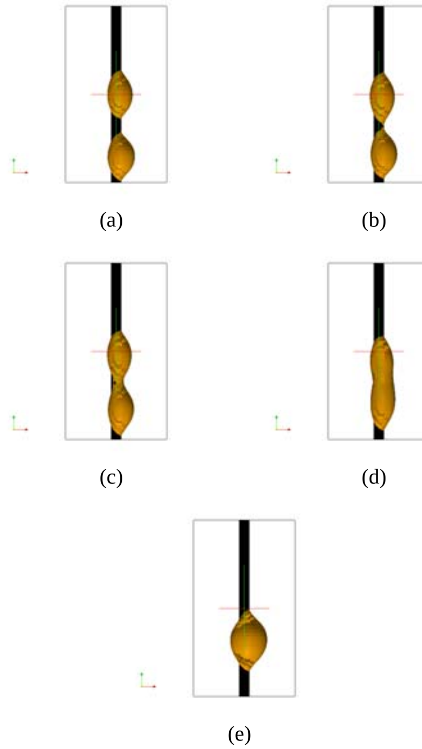
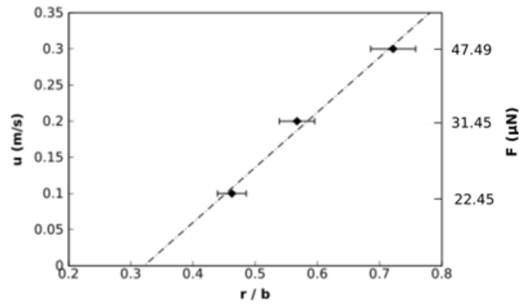


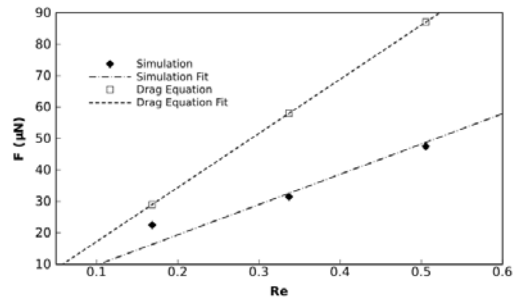
Figure 4: A series of images showing the movement of a coalesced droplet down a fiber under the influence of flow (u=0.2 m/s), and the merging of this droplet with the droplet immediately below

Both previous drag equations hold for low values of Reynolds' number (*Re*, *<1*); $Re = \frac{\rho u d_d}{\mu}$, where, ρ is the density of the fluid (air), d_d is the droplet diameter and μ is the fluid viscosity. The drag force of a "barrel" droplet on a fiber may then be approximated as $F_t = F_d - F_c$.

Fig. 5b shows the simulated forces acting on the droplets compared to the drag force on a sphere and cylinder. *Re* is plotted on the x-axis as this accounts for both u and b. The difference can be seen to become more pronounced as the velocity increases, most likely due to the simulated droplet not being truly spherical and also able to be deformed in the flow field, whereas in **??** the particle remains perfectly spherical. It is possible to obtain the relationship between F and *Re* and that between F and r/b from the linear fits shown in Fig. 5, such that; $F = 96.31Re$, and $F = 59.28\frac{r}{b}$. Thus, the force can be considered in terms of dimensionless parameters. Additionally, we can empirically derive an expression for r, such that; $r = 1.625bRe$, therefore, the droplet displacement may be found from the droplet size and flow parameters. This expression should hold for a range of droplet sizes, provided that the Reynolds number is low and the surface tension of the liquid similar. Previous work by Mullins et. al.[5] attempted to measure the force required to pull droplets off a fiber, however, these forces were significantly less than those simulated in the current work. Fig. 6 shows the



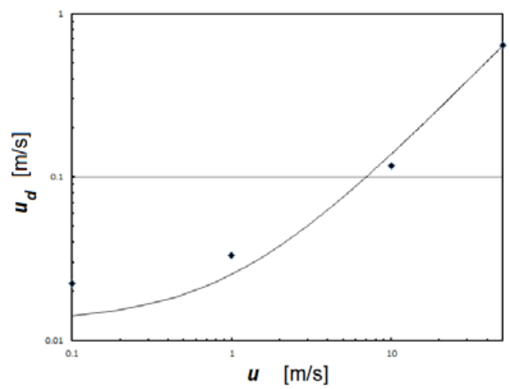
(a)



(b)

Figure 5: Forces calculated from results and F_t (a) shows the relationship between u, r/b and F for the simulations. (b) shows F obtained from the simulation and the drag equations against Re, the values shown are of a series of repeated simulations. The error bars on (a) indicated the error associated with measuring r and b from the simulation

(a)



(b)

Figure 6: (a) Re-entrainment of a droplet after axial motion at u=50 m.s^{-1}. (Airflow L-R parallel to fibre) (b) Droplet axial velocity u_d vs airflow velocity u (prior to re-entrainment)

re-entrainment of a 50 μm droplet after axial motion along the fibre, and a plot of the axial droplet velocity vs (parallel) airflow velocity. The forces simulated in the current work, however, are comparable with those predicted by the drag equations and of the same order of magnitude as forces measured on similar systems presented in the authors' previous work [1, 2]. Therefore we assert that the VOF solver can accurately simulate the forces acting on a liquid droplet.

Conclusions

This work has shown that it is possible to accurately simulate the break-up of a liquid film coating a cylinder under the influence of Plateau-Rayleigh instability. The VOF solver in OpenFOAM is able to simulate this break up based on solutions to the transport equations, without the need to develop detailed numerical models. The solver allows the force acting on the system at any point (e.g. the droplet surface, to be calculated). Realistic droplet displacement under the influence of the velocity field is also shown. Therefore, CFD can be seen as a valuable tool in the modelling of droplet-fiber systems [3], including more complex systems, or even completely disordered systems, such as mist filters. Furthermore, it has been shown that the OpenFOAM VOF can also resolve re-entrainment of liquid droplets from fibres and mist filters.

Acknowledgements

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