# Simulation of Bubble Bursting Leading to Droplet Formation

# R. Mead-Hunter<sup>1,2</sup>, M.M. Gumulya<sup>3</sup>, A.J.C. King<sup>1,4</sup> and B.J. Mullins<sup>1,2</sup>

<sup>1</sup>Fluid Dynamics Research Group, Curtin University, Perth, WA 6845, Australia

<sup>2</sup>Occupation and Environment, School of Public Health, Curtin University, Perth WA 6845, Australia

<sup>3</sup>Department of Chemical Engineering, Curtin University, Perth WA 6845, Australia

<sup>4</sup>Department of Mechanical Engineering, Curtin University, Perth WA 6845, Australia

### Abstract

Bubble bursting is one of the most common sources of atmospheric aerosols, and plays a role in a number of industrial applications. Bubble bursting has recently been proposed as one of the mechanisms by which oil collected by coalescing filters may become (re-) entrained in the gas phase, downstream of the filter. In this work we simulate the rise of a single bubble in a fluid, the bursting of that bubble, and the formation of droplets using OpenFOAM; and compare our results to existing data in the literature. This initial validation is used to determine key parameters of the system based on the dimensionless Morton number. Based on ours simulations and existing literature data we propose that there is a transition from a surface tension dominant regime to a viscosity dominant one at a viscosity to surface tension ration of 0.1.

## Introduction

The process of bubble bursting is responsible for the generation of a significant portion of atmospheric aerosols [4, 5]. This process occurs naturally on the ocean and other water surfaces. Bubble bursting also plays a role in a number of industrial applications, and is one of the mechanisms that may be responsible for the (re-)entrainment of collected liquid from coalescing filters [3].

The process being with the rise of s bubble through the liquid to the surface. At the interface, there will briefly exist a thin liquid film, separating the bubble from the air. This film then collapses, creating a cavity in the liquid surface, which surface tension will act to correct. This results in the rapid collapse of the cavity, producing a jet of liquid (liquid column) which rises and may eject a 'jet' drop, or series of 'jet' drops.

This process is much like the ejection of droplets from the rear of a coalescing filter, where, pools of liquid may form, with air breaking through the film, via the formation and subsequent bursting of bubbles on the film surface.

The Weber number (We), Bond number (Bo) and Morton number (Mo) are commonly used dimensionless terms which can be used to describe the dynamics of bubble bursting [1, 6]. These are defined as follows;

$$We = \frac{\rho V_{tip}^2 R}{\gamma} \tag{1}$$

$$Bo = \frac{\rho g R^2}{\gamma} \tag{2}$$

$$Mo = \frac{g\mu^4}{\rho\gamma^3} \tag{2}$$

where,  $\rho$  is the liquid density, R is the bubble radius,  $\gamma$  the liquid surface tension, g acceleration due to gravity,  $\mu$  the liquid viscosity and V<sub>tip</sub> is the tip velocity. The value of tip velocity, as used by Ghabache et al. [1] and in this work, is the velocity of the liquid column at the point where it reaches the surface of the bulk liquid.

These three dimensionless terms can be used to describe the dynamics of the ejection of 'jet' droplets as We is a function of Mo and Bo [1]. It is important to note that two relationships exist, as demonstrated in Figure 3 of Ghabache et al. [1] and Figure 4. The transition occurs at a value of Mo  $\approx 3 \times 10^{-8}$ , where the system transitions form a surface tension dominant regime to a viscosity dominant regime.

In his work we simulate the bubble bursting process and the subsequent formation of 'jet' droplets using the experimental data of Ghabache et al. [1] for the purposes of validation. If the key physical processes can be reliably captured then the simulation methods used can be more broadly applied to our coalescing filter case—an application where experiments are considerably more difficult.

The volume-of-fluid (VoF) method has previously been used to simulate bubble motion [6, 7] and to resolve the liquid interface on small scales [2] and will be applied here.

#### Methods

All simulations were conducted using the OpenFOAM software package (ESI Group). We utilised the volume-of-fluid (VoF) method to resolve the liquid-air interface, coupled with dynamic mesh refinement applied to all cells at the liquid-air interface (defined as cells with an alpha value of between 0.999 and 1).

Simulations were conducted in a rectangular domain, with a single bubble imposed below the liquid surface, and allowed to rise via buoyancy forces. Simulations were run for a time sufficient to allow the bubble to collapse, the liquid column to form and droplets to be ejected. Figure 1 illustrates the latter part of this process where several droplets have been ejected, form the collapsing liquid column. As the process is heavily dependent on the properties of the bulk liquid this time varied between simulations.

To ensure domain size did not influence the rise of the bubble or the behaviour at the interface a number of simulations were run to assess domain size. A domain width of 5 bubble diameters was found to be sufficient, with smaller widths resulting in unrealistic velocity profiles at the interface. These could otherwise be excluded by use of an appropriate domain size. Similarly, the level of mesh refinement required also needed to be explored, with insufficient refinement resulting in poor quality (and unrealistic) resolution of the interface, and excessive refinement significantly increasing the computational intensity of the simulations. An initial mesh comprised of 20 cells per bubble diameter was found to be sufficient.

Given the rapid nature of the bubble bursting process, a sufficiently small time step had to be used to ensure that the behaviour at the interface was properly captured. This was important to allow the tip velocity to be extracted. This parameter (as defined in Ghabache, et al. [1]), is the velocity of the rising liquid column at the point it reaches the height of the bulk liquid.

To allow comparison with the experiments conducted by Ghabache et al. [1], a number of different water-glycerol mixtures were simulated (water, and water with 20, 30, 40, 50, 55, 60 and 65% glycerol), which correspond to the range of Morton numbers found to produce 'jet' droplets on the break-up of the liquid column.



Figure 1. Simulated ejection of droplets following bubble bursting. The case shown is for a 2mm diameter bubble in a solution of 50% glycerol in water.

#### **Results and Discussion**

To examine the resolution of the liquid-air interface the results of simulations were compared visually to the images taken by Ghabache et al. [1]. For this 'visual validation' the simulations of 1 diameter bubbles in water and 50% glycerol solutions were used. The images shown in Figure 2, show the shape of the interface below the bulk liquid surface just before and just after the formation of the liquid column resulting from the collapse of the bubble. These compare favourably to the images shown in Figure 4 of Ghabache et al. [1].

The other important aspect in terms of resolving the interface is the ability to simulate the droplets ejected as part of the bubble collapse process. This is illustrated in Figure 3, for the bubble rising in water case. The expected behaviour (again with reference to the results of Ghabache et al. [1] can be seen, in terms of the ejection of the 'jet' drops and the ripples on the liquid surface.

The ability to resolve the interface is an important aspect of these simulations, however before such simulation can be applied to liquid (re-)entrainment in coalescing filters, we need to conduct a more quantitative analysis. This has been achieved by considering the tip velocity of the liquid column that results from the collapse of the bubble. By extracting this value from the simulations we were able to evaluate the values of We, Bo and Mo, as used by Ghabache et al. [1] we were able to plot the results of our simulations against their experimental results. These values are shown in Figure 4.





Figure 2. Profiles of the interface below the surface of the bulk liquid. (c) shows the final stage of bubble collapse, before the rise of the liquid column, designated  $t_0$ . (a) shows the profile at  $t = t_0 - 130 \ \mu$ s, (b) at  $t = t_0 - 30 \ \mu$ s, and (d) at  $t = t_0 + 30 \ \mu$ s.

There is reasonable agreement between the simulated values and the experimental values in Figure 4. It is important to note that where we have used bubbles o either 1 or 2 mm diameters in our simulations, Ghabache et al. [1] have used bubbles ranging from 300 to 2000  $\mu$ m. It is also evident form Figure 4, that our simulations have correctly captured the two different relationships with Morton number (as illustrated by considering the results either side of Mo =  $3 \times 10^{-8}$ ).

The differences observed between the 1 mm and 2 mm bubble diameter cases, also appear to be consistent, with the results for 2 mm bubbles constantly appearing above the results for the 1 mm bubbles. A trend easily explained by considering that both We and Bo are a function of bubble size. This also explains the vertical orientation of the results of Ghabache et al. [1], for liquids with the same value of Mo.

The range of Mo value covered by Ghabache et al. [1] appears to cover the range of liquid properties where 'jet' droplets are produced. Additional simulations on 80% glycerol and a multicomponent oil (Mo >  $1 \times 10^{-6}$ ) did not produce 'jet' drops, which would appear to assert this. Based on our simulations and the results of Ghabache et al. [1], we propose that there is a range

of Mo values where 'jet' drops may arise as a result of bubble bursting.



Figure 3. The ejection of droplets following the bursting of a single bubble in water. The image shows the first droplets being ejected 3.6 ms after the bubble has reached the liquid surface.



Figure 4. Comparison of the simulated results obtained for 1 and 2 mm diameter bubbles to the experimental results of Ghabache et al. [X]. The two different relationships with Morton number can clearly be seen, with the transition between these relationships occurring at  $Mo \approx 3 \times 10^{-8}$ .

This range starts with the low value of Morton number of the order of  $10^{-10}$  (that corresponding to water) and increase to a transition point at approximately  $3 \times 10^{-8}$ , where the viscosity dominant regime takes over. 'Jet' droplets still form under this regime, however the velocity with which they are ejected appears to decrease, to a point where the collapse of the liquid cavity, does not give rise to droplets. Based on our simulations, this region occurs in Morton numbers between  $1 \times 10^{-6}$  and  $1 \times 10^{-5}$ .

Given that the Morton number is heavily dependent on the surface tension and viscosity of the liquid, it may also meaningful to consider these two parameters alone. If we choose the viscosity to surface tension ratio ( $\mu/\gamma$ ) then our region of transition between the surface tension dominant regime (left of Mo = 3 × 10<sup>-8</sup> in Figure 4) and the viscosity dominant regime (right of Mo = 3 × 10<sup>-8</sup> in Figure 4) occurs at approximately  $\mu/\gamma = 0.1$ , our region where we no longer get 'jet' droplets formed corresponds to approximately  $\mu/\gamma = 0.2$ . Broader application of such limits would require further simulations of additional liquids, with properties around these limits.

In terms of coalescing filters, is appears that we will be able to simulate the fundamental processes relating to droplet (re-)entrainment, however our results here appear to indicate that the use of a rising bubble in a liquid column as an analogue may be limited. Calculation of the Mo and  $\mu/\gamma$  values for di-ethyl-hexyl-sebacate (DEHS) results in values of  $1.2 \times 10^{-4}$  and 0.77, respectively—outside our proposed range for 'jet' droplet formation. The formation of 'jet' droplets from the rear of coalescing filters may therefore also be dependent on localised flow velocities of air through the filter, or potentially another mechanism.

### Conclusions

We have found that with an appropriate level of dynamic mesh refinement, we can simulate the bubble bursting process and the formation and ejection of 'jet' droplets. It can be seen that this process is heavily governed by the Morton number and that there are surface tension dominant and viscosity dominant regimes, with the transition between the two occurring at a Morton number of approximately  $3 \times 10^{-8}$ . This corresponds to a viscosity to surface tension ratio of 0.1 for the liquids simulated.

Based on our results it should be possible to simulate the bubble bursting processes that result in the (re-)entrainment of larger droplets form coalescing filters. However, any extrapolation of relationships that exist the bubble rise case may not be physically meaningful, due to the differing dynamics.

## References

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