Simulations of Drop Break-Up

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Abstract
Numerical simulations of the break-up of falling liquid drops are performed using an adaptive $hp$-finite element method. Results show the initial stages of the “bag” phenomenon which leads to break-up. Because of the increased frontal area which occurs as the drops deform, the drag increases and there is a maximum in the drop velocity. This maximum velocity was used to determine a critical Weber number of break-up. Comparing the critical Weber number at various conditions, it was found that it is insensitive to the Ohnesorge number but mildly sensitive to the liquid-to-gas density ratio. Drops with a smaller density ratio have a lower critical Weber number. Lastly, it was postulated that drops near break-up do not respond in a quasi-steady manner to the flow rather there is a time history effect. This postulate is based on the fact that during the drop evolution we observed two very different drop shapes at the same slip velocity.

Introduction
Accurately predicting the conditions at which a drop breaks up is critical for capturing the dynamics of a spray. Break-up increases the surface-to-volume ratio of the spray and thus dramatically impacts surface phenomena such as the total drag on the spray and its net evaporation rate. These are the primary phenomena that determine where and at what rate liquid fuel is converted to gas. As such, for reliable predictions of combustor performance, break-up must be well understood and modeled.

To this point, most information on drop break-up has come from either drop-tower or shock-tube experiments [1]. There has been little information obtained from either analytic solutions or numerical simulations. Because break-up is such a non-linear phenomenon, analysis techniques have not been very successful. Likewise, numerical techniques have typically had difficulty providing reliable results for this phenomena. This is because the phenomenon is highly sensitive to perturbation and it is difficult to perform an accurate calculation for problems with a highly convoluted interface. High-accuracy techniques such as the arbitrary-Lagrangian-Eulerian approach (ALE) are usually limited to low or moderate interface deformation.

Recently, we have developed an adaptive ALE approach [2] that provides high-accuracy results even for problems with highly convoluted interfaces. This approach allows us to perform detailed simulations of drop break-up and thus obtain information that is difficult or impossible to obtain from experiments. Furthermore unlike an experiment, we have complete control of all of the parameters of the simulation, and can precisely investigate the effect of each parameter on the onset of drop break-up. Lastly, it is well known that drops are extremely sensitive to surface contaminants [3]. In an experiment it is usually very difficult to characterize the degree of contamination of the drops. By performing simulations of contaminant-free drops, we can bound this limit of drop behavior.

In the following, we report on several preliminary simulations of drop break-up. At this point, we have only begun to investigate the parameter space, but in spite of this, we have found new phenomena which have not been discovered from experimental data. These phenomena are discussed and the implications for predicting drop break-up are analyzed.

Formulation
The problem is that of a liquid drop accelerating from rest through a stationary gas. The fluids are assumed to be incompressible and are separated by a surface with a constant surface tension, $\sigma$. The liquid and gas are assumed to have constant densities, $\rho_l$ and $\rho_g$, and viscosities, $\mu_l$ and $\mu_g$, and the drop accelerates under a volumetric force with acceleration constant $g$ (i.e. gravity). This problem exactly mimics a drop-tower experiment. The simulations are axisymmetric and for the simulations presented here, the terminal Reynolds number, $Re = \rho_g Ud/\mu_g$ where $U$ is the drop’s terminal velocity and $d$ is the
drop diameter, is below 200. Above $Re = 200$, it has been shown that flow over a solid sphere becomes non-axisymmetric [4]. Although we keep the Reynolds number below 200, there is still the possibility of a non-axisymmetric instability for drops. However, experimental data has shown that in the initial periods of break-up the drops remain fairly axisymmetric [5]. Thus the phenomenon at least initially is not influenced by non-axisymmetric effects.

The applied body force accelerates the drop through the flow until it either reaches a steady terminal state or it breaks-up. Since we are interested in studying break-up, we set the magnitude of this force such that the drop breaks-up before reaching its terminal velocity. The magnitude of force needed is estimated from drag correlations for a solid sphere with the requirement that at the terminal velocity the Weber number, $We = \frac{\rho d U^2}{\sigma}$ be approximately 25. The other parameters in the problem are the density ratio, the viscosity ratio, and the Ohnesorge number, $Oh = \frac{\mu}{\sqrt{\rho \sigma d}}$. In this work, we perform some preliminary investigations of the effect of density ratio and the Ohnesorge number on break-up. We have not yet examined the effect of viscosity ratio. For the results presented here the viscosity ratio is always 10.0.

The simulations are performed using an $hp$-finite element method [6]. In this method, an unstructured mesh of triangles is used which deforms with the interface. This allows higher-order accuracy to be obtained even though there is a discontinuity at the interface. On each triangle, fourth-order polynomials are used to represent the solution. This gives a higher-order of spatial accuracy (5th order). The difficulty with this approach is that as the drop approaches break-up the mesh becomes highly-deformed and eventually unusable. This difficulty is overcome by implementing a dynamic mesh adaptation algorithm [2, 7]. The adaptation algorithm simultaneously allows large deformation problems to be simulated and also maintains an appropriate mesh resolution for resolving the features of the solution. This allows accurate simulations to be performed even when the drop develops localized regions of high-curvature. This is shown in the results section. The main limitation of this approach is that topological reconnection of the surfaces can not be simulated. As such, the simulations can only be performed up to the point of break-up. We show in the results section that this does not hamper our ability to predict the critical Weber number of break-up.

All of the results presented are calculated on a trapezoidal domain given by the $r, z$ points $(0, -10)$, $(0, 15)$, $(10, 7.5)$, and $(10, 12.5)$ with the drop positioned at $r, z = (0, 0)$ where the units are drop diameters. In [8], we have shown that with this boundary distance, the drag on a solid sphere is accurate to within 1% for a Reynolds number of 100. However we have recently found that for Reynolds numbers less than one, the boundaries should be farther away. For the results shown here, the terminal Reynolds numbers are above 20 so there still should be little sensitivity to boundary conditions.

**Results**

The results of three specific cases are studied. These are for the conditions listed in table 1. The body force is given in terms of the Eotvos number, $Eo = \frac{\rho gd^2}{\sigma}$. In physical parameters, changing from the first case to the second case corresponds to a change in liquid density while the liquid and gas viscosities, and drop size are held constant. The gravitational force is varied in inverse proportion to the liquid density to maintain nearly the same terminal Weber number. Changing from the first case to the third case corresponds to a change in diameter of the drop while holding the liquid and gas properties constant. The gravitational force is adjusted to maintain the same terminal Weber number. All of the drops studied tend to become oblate as they fall. In [8] we have shown that for some conditions an axisymmetric drop can become prolate. We have excluded these conditions from the study because prolate drops are not axisymmetrically stable and thus the results will not be physically relevant.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\rho_l/\rho_g$</th>
<th>$\mu_l/\mu_g$</th>
<th>$Oh$</th>
<th>$Eo$</th>
</tr>
</thead>
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<td>50</td>
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<td>60.0</td>
</tr>
<tr>
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<td>5</td>
<td>10</td>
<td>1.0</td>
<td>60.0</td>
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<tr>
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<td>50</td>
<td>10</td>
<td>0.1</td>
<td>33.3</td>
</tr>
</tbody>
</table>

Table 1: Simulation conditions.

Figure 1 shows the drop shape for Case 1 at a time near break-up. The left side of the figure shows the computational resolution to demonstrate the accuracy of the calculation. The right side of the figure shows the vertical velocity contours and drop shape. From the figure, we see similarity to a “bag” break-up phenomena [5, 9]. The drop mass moves to a ring away from the centerline leaving a thin sheet of fluid across the centerline. This is a direct resultant of the gas-phase pressures on the drop. In a frame moving with the drop, there are higher flow velocities around the equator of the drop, thus the pressure is low at the equator. This draws the drop into an oblate shape. As the drop approaches break-
up, this distortion continues until we arrive at the shape shown in figure 1.

To determine a critical Weber number, we plot the instantaneous Weber number based on the slip velocity of the drop versus time. Time is non-dimensionalized by the inviscid oscillation time associated with a free drop, $\sqrt{\rho l d^3/\sigma}$. Initially the velocity increases linearly with time which is the quadratic portion of the curve since the Weber number is proportional to velocity squared. After a time, $t$, of 500, the drag on the drop begins to play a role and the rate of increase in velocity decreases. If the drop were not going to break-up, we would see an exponential convergence to the drops terminal velocity. Instead, we see a surprising phenomena. Because of the increase in the drop’s frontal area as the Weber number increases, the drop actually slows down. This leads to a maximum in the Weber number versus time. We use this maximum to unambiguously define the critical Weber number. For this case, we find that the maximum Weber number is 20.4 which is in good agreement with experimental data. Results from Hsiang and Faeith [1] estimate that the transition to bag break-up is between $We = 1$ and 20.

It is interesting to note that the drop does not respond in a quasi-steady manner to the slip velocity; There is a strong time history effect. This is apparent because there are two different drop shapes at the same Weber number. For $We = 19.2$, one is moderately deformed with an aspect ratio of 0.16 occurring at $t = 1000$ and the other is highly deformed with an aspect ratio of 0.03 occurring at $t = 1375$. The aspect ratio here is defined as the centerline length of the drop divided by the maximum diameter of the drop. We have shown in [8] that based on scaling arguments the quasi-steady assumption is reasonable for these conditions, however these results indicate that this assumption is not valid near break-up. Since the evolution is occurring over many drop oscillation periods, we postulate that it is not the drop response based on surface tension but rather the momentum of the liquid moving in the radial direction which is causing the non quasi-steady response.

To determine the effect of liquid density on the critical Weber number of break-up, we repeat the above experiment for Case 2 in table 1. As mentioned previously, this corresponds to essentially the same terminal conditions in terms of Weber number and Reynolds number, the only difference is the density of the liquid. Figure 3 shows the drop shape near break-up. Again we see a similar shape with a ring of liquid connected by a thin sheet. Figure 4 shows the time history of the Weber number. In this case the evolution occurs over fewer drop oscillation times than in the previous case. The reason for this is that in order to maintain the same net body force the gravitational acceleration must be increased when the liquid density is decreased. The change in drop oscillation time with density is less significant because it is a square root dependence. Figure 1.

From figure 4, we again see that the Weber num-
Figure 3: Mesh resolution and vertical velocity contours for Case 2.

Figure 4: Weber number based on instantaneous slip velocity versus oscillation time for Case 2.

Figure 5: Mesh resolution and vertical velocity contours for Case 3.

The Weber number reaches a maximum. In this case, the maximum is 16.9. Thus lower density drops break-up at a lower Weber number. We have not been able to determine whether this is in agreement with experimental findings because it is difficult to find pairs of fluids for which the density ratio changes while the viscosity ratio remains fixed.

The last case is for the same fluid properties as Case 1, but a different Ohnesorge number. This basically corresponds to changing the drop diameter. Figure 5 shows the drop shape near break-up. In this case, we the drop is even more stretched than the previous cases, but the general shape is the same. Figure 6 shows the time history of the Weber number. Again we see the Weber reaches a critical value then decreases. The maximum Weber number is 21.0 which is very close to that predicted from Case I (20.4). Although the Ohnesorge number only changes from 0.3 to 0.1, this corresponds to almost a factor of 10 change in drop diameter. Thus for this range of conditions, the critical Weber number is insensitive to drop size. This is in agreement with experiments which show that when the Ohnesorge number is less than 1, the critical Weber number is nearly independent of $Oh$ [1].

Conclusions
We have performed several preliminary simulations of the break-up of liquid drops. For all of the cases studied, we see a “bag” break-up phenomenon in which a ring of liquid forms with a thin sheet across the center of the ring. Because of the increased
frontal area of this shape, the drop reaches a maximum velocity then slows down. This maximum velocity was used to define a critical Weber number of break-up. These preliminary results show that the drops are very weakly sensitive to the Ohnesorge number and only mildly sensitive to the liquid to gas density ratio. Another important finding is that the drops do not respond in a quasi-steady manner to the flow. This means that the break-up behavior of drops will be strongly sensitive to the time history of the flow leading to break-up. Further investigations are needed at a wider range of conditions and also to investigate the importance of flow time history on break-up. This can be done by comparing these unsteady solutions to either quasi-steady results or results with different acceleration rates.

References


