Detailed Understanding of Drop Atomization by Gas Crossflow Using the Volume of Fluid Method

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Abstract
Two popular yet conflicting theories exist in the atomization community to describe the breakup of a liquid drop by gas crossflow: 1) the ‘shear’ or ‘boundary-layer stripping’ theory and 2) the surface waves driven, sheet atomization theory. Various compelling arguments have been put forth in support of both theories, but there has been no authoritative conclusion on the validity of either one. In this paper, we present detailed understanding of liquid drop breakup by gas crossflow using the Volume Of Fluid (VOF) approach, a computational method that tracks the liquid-gas interface. The VOF approach is first compared and validated against existing experimental data for liquid drop breakup. Then, detailed insights are provided for the drop breakup process using VOF. Substantial evidence is presented to help resolve the debate on drop breakup phenomenological theories.

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Introduction

The breakup of a single liquid drop by gas crossflow is of fundamental importance in many combustion systems. The rate of atomization and evaporation of liquid drops significantly affects the combustion efficiency in gas turbine engines, augmentors, diesel engines and many practical applications. The mechanisms leading to liquid drop breakup have been extensively studied experimentally and theoretically for many years. Multiple and often conflicting phenomenological models have often been proposed to describe the drop breakup process. Unfortunately, definitive understanding on the processes leading to the breakup of a liquid drop by gas crossflow has been elusive to date.

There exist at least two different, popular theories that explain the breakup of a liquid drop in the shear breakup regime: 1) The boundary-layer stripping theory originally proposed by Ranger and Nicholls [1] and 2) the surface waves driven, sheet breakup theory originally proposed by Liu and Reitz [2].

The boundary-layer stripping theory has had quite a backing from the academic and industrial community since Ranger and Nicholls [1] first published it. Ranger and Nicholls [1] proposed that a drop breaks into smaller drops when the shear action of air strips of some mass from the boundary layer on the liquid drop. Figure 1 shows a schematic of the boundary layer stripping proposition and an example experimental picture that is used to justify the same. The theory proposes that liquid material is continuously stripped off from the surface of the drop till the drop is reduced to a fine micro-mist.

Many researchers have used a boundary layer analyses to develop correlations for the rate of disintegration of the parent drop, SMD and velocities of child drops etc. A significant amount of experimental and theoretical research has been carried out by Professor Faeth’s group supporting the theory of boundary layer stripping as the main cause of drop atomization. Hsiang and Faeth [3] studied the breakup of a liquid drop to determine the various regimes of drop breakup (bag, multimode, shear etc.) as a function of Weber number and Ohnesorge number. Drag coefficient as a function of drop deformation and shearing were noted, and drop size correlations of child drops resulting from the parent drop’s breakup were developed based on the boundary layer stripping theory. Chou et al. [4] developed correlations for rate of liquid removal and child drop SMD and velocities as a function of the parent drop’s lifetime based on the boundary layer stripping theory in the shear breakup regime. Various prominent research groups have also supported the boundary layer stripping theory as the mechanism responsible for liquid drop breakup, Delplanque and Sirignano [5], Wierzb and Takayama [6] and Chryssakis and Assanis [7] to name a few.

The surface waves driven, sheet atomization theory originally proposed by Liu and Reitz [2] attributes the breakup of liquid drops to be caused by unstable waves growing on the surface of the drops. Liu and Reitz [2] analyzed the distortion and breakup mechanisms of high-speed liquid drop and showed experimental evidence in support of a dominant sheet based breakup mechanism. It was observed that the drop flattens and deforms into a convex sheet in the shear breakup regime due to aerodynamic forces. The breakup of the convex sheet then occurs by a mechanism similar to the ‘stretched streamwise ligament’ breakup mechanism described by Stapper and Samuelsen [14]. Lee and Reitz [8] studied the effect of liquid properties on the breakup mechanism of high-speed liquid drops supporting sheet based atomization and casting more doubt on the existence of the boundary layer stripping mechanism. Various research groups have also endorsed “waves driven” atomization as the primary cause of drop breakup, with different approaches such as TAB (O’Rourke and Amsden, [9]) and ETAB (Tanner [10], [11]).

The primary points to be taken from several of the studies on liquid drop atomization are that (a) the mechanisms leading to drop breakup are still unclear and (b) considerable difference of opinion exists within prominent research groups across the world on the processes leading to drop breakup. The objective of the present work was to investigate the breakup mechanisms of liquid drops by gas crossflow by employing a high fidelity numerical approach – Volume Of Fluid (VOF). The benefits of a high fidelity numerical approach become very evident in this situation as no definitive conclusion can be arrived at by experimental observations alone. To our knowledge, the VOF approach has not been validated and used so far to provide detailed insights into the drop breakup process by gas crossflow. This paper describes the computational approach used to employ VOF to study drop atomization, and presents detailed insights into the drop breakup processes in the bag and shear breakup regime.

Volume Of Fluid Method

The Volume Of Fluid (VOF) technique proposed by Nichols and Hert [12] is typically used for tracking the motion of free surfaces. In VOF, a scalar quantity \( f \) is defined that represents the fraction of the volume of a mesh cell occupied by one phase, say the liquid. Thus for \( f = 1 \), the mesh cell is entirely filled with liquid, while for \( f = 0 \) the mesh cell is entirely filled with gas. In a mesh cell that instantaneously contains a part of the interface both phases coexist and \( 0 < f < 1 \). The strength of the VOF approach lies in the fact that highly irregular liquid gas interfaces can be represented accurately.

Since liquid volume is conserved, the liquid volume fraction, \( f \) in each cell can be computed numeri-
CFD Problem Specification

The breakup of a single liquid drop by gas crossflow is usually studied with the help of a shock tube experiment (Nicholls and Ranger [1], Hsiang and Faeth, [3], Chou et al. [4]). The shock tube setup consists of a single liquid drop placed in the low-pressure side of the tube. When the diaphragm is broken, a shock passes through the low-pressure side and sets up a uniform flow field almost instantaneously. The drop then deforms and breaks based on the flow field and observations are made regarding the breakup processes by employing various visual aids (Figure 2).

Simulating the entire shock tube experiment to study the liquid drop breakup using the VOF method in 3D will result in hundreds of millions of cells and make the computation completely impractical. An engineering approach is needed with VOF to analyze liquid drop breakup that allows accurate and reliable analyses while still remaining computationally practical.

The first element in cost reduction that we investigated was the suitability of a “reduced 3D” or 2D axis-symmetric computation as compared to the full 3D simulation. Since, as of now, we are primarily interested in just the processes leading to drop breakup and not the characteristics of the resulting drops, we can justify using 2D axis-symmetric or simplified 3D simulations. Figure 3 shows a close-up on the three cases that were analyzed to reduce the computational expense as compared to a full 3D case. Figure 3(a) shows the full 3D case, Figure 3(b) shows the reduced 3D case where we analyzed only a quarter of the drop by employing symmetry boundary conditions at the quarters, Figure 3(c) shows the 2D axis-symmetric case. The full 3D case had approximately 7 million cells, the reduced 3D case had approximately 2 million cells and the 2D axis-symmetric case had less than 100,000 cells. Figure 4 shows the time history of the breakup process in all the three cases by showing the volume fraction of the liquid at the center plane of the drop. The breakup process is very similar in all the three cases, thus demonstrating that the mechanisms responsible for liquid drop breakup can be computed numerically in a 2D axis-symmetric sense. The 2D axis-symmetric feature of the drop breakup process makes the numerical analysis using VOF highly feasible. A similar analysis as above (3D versus reduced 3D and 2D axis-symmetric) was carried out at various Weber number conditions to ensure the suitability of 2D axis-symmetric assumption in the bag and shear breakup regimes.

Although doing 2D axis-symmetric simulations are economical as compared to full 3D simulations, an extensive parametric study of the 2D axis-symmetric full shock tube experiment is still not very efficient. Simulating the entire shock tube experiment is rather time consuming for a parametric study because of (a) the increase in the cell count that comes from simulating the entire shock tube and (b) the decrease in time step size that is needed to resolve the shock motion through the computational domain. Thus to further reduce the cost from our CFD setup while still preserving acceptable accuracy levels, we decided to build even simpler cases. The goal was to simulate the shock tube conditions in a smaller 2D axis-symmetric case with boundary conditions that allow us to “simulate” the shock rather than actually resolve it.

First we performed an entire shock tube CFD calculation to build a benchmark for the flow field features in the shock tube environment. Such a benchmark would help build low cost CFD cases that mimic the important characteristics that we are interested in simulating. Figure 5 shows a part of the computational grid used to simulate the shock tube experiment of Chou et al. [4]. The driver section was 3.1 m long and the driven section was 6.7 m long with the drop location 4 m from the downstream end. The grid was refined near the region where the drop existed and the atomization processes would be dominant. The total cells in the shock tube grid were roughly 370,000 (2D axis-symmetric analysis). Figure 6 shows a time sequence of the breakup processes observed in the shock tube case. The shock passes by the drop and a flow field is setup instantaneously. There are no observable, significant pressure fluctuations, and the flow field is practically uniform throughout the drop breakup process. A recirculation zone forms behind the drop and expands trans-
versely as the drop starts to distort. The drop does not deform due to the shock wave at all. It’s the flow field behind the shock that causes the deformation and disintegration (which is consistent with experimental observations (Figure 2)). Now the goal was to setup a CFD case that would replicate such flow field characteristics as closely as possible.

Two different choices exist to simulate the shock tube experiment in a reduced grid without actually resolving the shock: 1) the drop can be placed in a quiescent environment and a fixed velocity boundary condition can be specified at the inlet according to the desired Weber number, or 2) the drop can be placed in a quiescent environment by creating a special grid just around the drop and the rest of the flow field can be initialized by the inlet velocity according to the desired Weber number. Because of limitations in the VOF problem specification in CFD-ACE+, we could not directly specify the drop to be at zero velocity and the rest of the domain to the inlet velocity. Thus, the second option was an attempt to as closely achieve the effect of zero velocity drop and rest of the domain at inlet velocity. Our approach here was to simulate the shock tube experiment most closely by setting artificial boundary conditions and initial conditions on a much smaller grid than the one used for the shock tube simulation. Figure 7 shows these two options for setting up the CFD case to simulate the drop breakup. Both these options have less than 100,000 cells. Figure 8 shows how the flow develops in time in the computational domain for each of the cases. The case where the whole domain was initialized to zero velocity shows significant pressure pulsations in the beginning and takes approximately 100 times more computational time for the flow to settle down to a state which is representative of the shock tube experiment. The case where only the domain close to the drop was initialized to zero and the remaining domain was initialized to the inlet velocity, settles down very quickly and matches the shock tube flow profiles much more closely. Based on this analysis, we decided to use the latter option for further liquid drop breakup CFD cases. Sufficient testing was also done for the drop placement in the computational domain to ensure that there is no artificial interaction between the drop and the boundaries. It was found that the inlet boundary had to be at least five drop diameters upstream of the drop to avoid interference by the inlet boundary.

A grid dependence check was also done to ensure that the important breakup mechanisms are well resolved. Figure 9 shows the comparison between grids of resolutions going from a uniform 30 micron cell size to 5 micron cell size for a parent drop of the size of 600 microns. The 5 to 12.7 micron grids produced nearly identical breakup times and spread, and provided fine enough resolution to capture the breakup processes. The 30 micron cell size produced different results and was considered unsuitable for the VOF calculations. At the Reynolds numbers considered in this work, the grid with 10 micron cell size provided at least 6 cells in the liquid boundary layer on the drop. Thus we ensured that the boundary layer effects are well captured for the CFD.

Based on the analysis presented in this section, it was decided to perform a CFD analysis with the following properties:

a) 2D axis-symmetric, compressible flow
b) Zero initial velocity domain around the drop
c) Uniform velocity at inlet and around the drop
d) 10 micron cell size resolution

The following section discusses the validation of the VOF approach for liquid drop breakup by gas cross-flow. The drop considered in the work presented in this paper is a 600 micron ethanol drop unless specified otherwise.

Validation of VOF for Liquid Drop Breakup

Experiments have noted two very distinct breakup mechanisms at low and high Weber number conditions viz. the bag breakup and shear breakup respectively. In the bag type breakup mode, the drop deforms to form a bag type structure at its core before it disintegrates into smaller drops (Figure 10a). In the shear breakup mode, the drop starts breaking from its edges and slowly disintegrates into a micromist (Figure 10b). Regardless of the “phenomenological theory” that describes the breakup process, the bag breakup is observed in low Weber number conditions, usually between 10-30 and the shear breakup mode is observed at high Weber number conditions, which are typically above 60. Figure 11 and 12 show that VOF correctly predicts the bag and shear breakup regimes in the experimentally observed Weber number conditions of 15 and 81 respectively. A parametric set of cases was run to vary the Weber number from 10 to 150 by changing the initial conditions and the inlet flow conditions while keeping the drop size constant at 600 microns. Dai and Faeth [13] performed a similar parametric study to analyze the characteristics of drop breakup as a function of Weber number experimentally. Figure 13 shows a comparison of the onset of breakup as calculated by VOF and observed in experiments of Dai and Faeth [13]. The qualitative trend of the onset of breakup is very well captured by the VOF calculations. However, there exists a constant difference in the predictions of normalized time. The difference in CFD predictions and experimental results can be attributed to the hazy definition of t = 0s. In the CFD calculations, time was initialized to zero at the beginning of the calculations where the shock is already assumed to exist. While in experiments, the time could have been initialized when the diaphragm was broken or based on some other metric.
Figure 2 shows experimental snapshots of a shock going over a liquid drop by Rachner and Nicholls [1]. It can be clearly seen that the time when the shock goes over the drop is non-zero. Such could have easily been the case in the study of Dai and Faeth [13] also. Thus the initialization of time to zero could explain the discrepancy that we see in the onset of drop breakup.

Table 1 compares CFD results with experimental observations on the occurrence of various regimes and onset of breakup in the different regimes. The VOF calculations correctly capture the various trends observed in experiments. Figure 14 shows the drop behavior at an instant of time as the Weber number is increased. In all the breakup regimes, the drop first deforms to form a thin disk like structure. In the bag breakup regimes the central portion of the drop moves faster than the edges to form a bag like structure, while in the shear regimes, the edges move faster than the central portion creating an appearance of shearing. Technically however, we did not observe any “boundary-layer” shearing. The refinement was fine enough to capture the boundary layer at the Reynolds numbers considered, but it was not the boundary layer that got sheared, but the entire edge itself. Development of surface waves on the edges of the flattened drop were clearly observed which resulted in the shearing/stripping away of the entire edge.

As shown above through Figures 11-14 and Table 1, the VOF calculations matched very well with the qualitative and quantitative trends of experiments. To build more insight and reliability on the breakup process, the effect of Reynolds number, different drop sizes and different liquids was considered with VOF calculations. Figure 15 shows a case where the Reynolds number was varied by changing the size of the drop. The Weber number was maintained at a constant value of 45. Both the drops underwent a similar breakup process, indicating that the liquid drop breakup is not a function of Reynolds number in the regime considered, but only the Weber number. To further verify this fact, the liquid of the drop was changed from water to ethanol while preserving the Weber number in a different regime (We=15, bag breakup regime). The drops underwent almost identical breakup processes again concurring to the experimental observations that the liquid breakup is a function of the Weber number rather than the Reynolds number (Dai and Faeth [13]).

The validity of VOF was further analyzed by comparing the ratio of maximum drop diameter and original drop diameter with the change in Weber number. Figure 16 shows the comparison of the VOF calculations and the experimental data of Dai and Faeth [13]. Similar trends were observed in the computational and experimental observations. The ratio of the maximum drop diameter and the original drop diameter practically remains constant throughout the breakup regime for We > 20. The CFD calculations predicted the ratio to be constant at ~ 3.5 while the experiments noted the ratio to be ~ 2. The discrepancy in this observation was attributed to the unclear definition of the maximum drop size. The drop deforms into a disk like shape and further bends into a conical sheet before the breakup of smaller drops is actually observed. In CFD we defined the maximum drop diameter to be the size from the center to the edge when the child drops are stripped from the edges in the shear breakup regime. However, the maximum drop diameter measurement metric could have been different in the experiments. Nonetheless VOF does predict the experimentally observed trends correctly.

The time history of the parent drop trajectories from VOF calculations was compared with the theoretical-experimental observations of Chou et al. [4]. The VOF calculations could accurately predict the qualitative trends in the drop trajectories. The path and rate of change of the drop path from the CFD results were copasetic with the experimental observations.

Overall, the validity of using VOF for liquid drop breakup is well established by the comparisons presented above. VOF is demonstrated to be a reliable, predictive tool to understand the breakup of a liquid drops by gas crossflow and holds the promise of providing insights into the drop breakup process that are hard to obtain from experiments alone.

**Using VOF to Understand Drop Breakup**

Figures 9, 12, 14 and 15 show different instances of the shear breakup process observed in VOF simulations and Figures 4 and 11 show different instances of the bag breakup process. In both breakup modes, the drop first deforms to form a disk like structure (Figure 18). Experimentalists have also observed that the drop deforms to form a disk like structure before the liquid mass removal starts (Pilch and Erdman [15], Wierzba and Takayama [6], Liu and Reitz [2]). The interpretation of the breakup process after the disk-shaped drop has been formed is the most controversial in the history of drop atomization understanding and has lead to bifurcation of the phenomenological theories.

The boundary-layer-stripping sect of our community believes that the boundary layer around the drop is what will strip off and remove mass from the parent drop. On the other hand, the surface wave driven, sheet atomization sect believes that the drop further deforms into a conical sheet and the edges break off due to wave growth on the windward side of the sheet.

It can be clearly seen in the VOF numerical experiments that the drop deforms to form a conical sheet and the sheet breaks up to remove mass from the parent drop. It is emphasized here that sufficient effort was made to resolve the boundary layer on the liquid drop. At times the grid resolutions was more than 10 times
finer than the boundary layer thickness at the Reynolds numbers considered.

At low velocities, the pressure in front of the drop at the stagnation point is more than the pressure at the back side of the drop. This pressure differential drives the drop to form a disk and then continues to form a bag before the drop disintegrates into smaller drops. At sufficiently higher velocities however, the drag/shear stress from the flow field causes the liquid in the drop to move faster from the center of the drop to its edges. As the round drop deforms to form a disk shape, the liquid at the edges is traveling faster than its central core. Although the pressure differential across the drop is trying to deform the drop to a bag shape, the velocities on the edges of the liquid drop are high enough to form a convex, conical shaped drop. Once the conical shape is formed, the edges strip off. This breakup could potentially be modeled using conical sheet breakup theories.

Thus the two competing effects in the liquid drop breakup by gas crossflow are: 1) the pressure differential across the drop trying to cause the drop to form a concave (bag-like) breakup and 2) the drag from the air flow field that accelerates the windward side liquid surface to go to the edges and continue on to form a convex shape. The pressure differential will cause the drop to form a disk like structure. If the speed of the windward side liquid on the drop surface is fast enough, the drop will deform into a convex shape, else it will break via the concave (bag-like) process. When the strength of these opposing forces is nearly equal, the “multi-mode” breakup can happen.

We performed 3D VOF calculations of the drop breakup process to further understand the breakup development. Figures 19 and 20 show the 3D VOF simulation time sequences of the bag and the shear breakup modes. It can be clearly seen that the drop deforms into a flat disk like shape and enters the bag breakup mode for low speed flows where the pressure effects dominate, and the shear breakup mode where the windward liquid surface velocity dominates. Figure 21 shows some experimental pictures against CFD snapshots to indicate how CFD reflects what is seen in experiments, but can provide much more detailed insights so that the experimental pictures are better interpreted. Thus we can see how viscosity of the liquid, speed of the air, surface tension of the liquid and density of the liquid will combine to play an important role in the breakup process. Traditionally, these effects have been lumped together in non-dimensional numbers of Weber number, Reynolds number and Ohnesorge number. Correlations between these numbers can be developed using VOF to come up with simplistic models for liquid drop breakup. While simultaneously, VOF can help build and validate sophisticated sheet breakup theories for detailed drop breakup models.

**Conclusion**

A VOF based computational approach was validated and used to provide detailed insights into the breakup of a liquid drop by gas crossflow. The breakup of a liquid drop by gas crossflow was found to follow the surface wave driven, sheet breakup mechanism instead of the boundary-layer stripping mechanism. It was demonstrated that VOF can be successfully used to obtained detailed information on the atomization behavior of a liquid drop breakup by gas crossflow. VOF provides a detailed and more controlled environment to study fundamental processes and can help further our understanding in the liquid atomization process like dense spray regions and jet in crossflow atomization applications. Although not demonstrated in this paper, VOF can provide enough information on the breakup process to build reduced models and design rules for practical applications. With the confidence gained in the VOF capability to predict liquid atomization, we are focusing future efforts on understanding near-field liquid jet breakup by gas crossflow. Figure 22 shows a 12.5 million cell VOF calculation of a liquid jet in cross-flow. Such simulations take 2-3 weeks to run on 15 processors, but provide detailed insights into the jet breakup mechanism and near-field dense spray region.

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Dr. Sam Lowery from CFDRC provided valuable guidance on the use of VOF throughout our research activity. CFDRC Internal R&D support funded this research effort and the authors would like to thank CFDRC for their support.

**Nomenclature**

\[ d \quad \text{diameter of the liquid jet/column} \]

\[ Re \quad \text{Reynolds number } \left( \rho_{\text{g}} d \mu_{\text{g}} / \mu_{\text{g}} \right) \]

\[ SMD \quad \text{Sauter Mean Diameter} \]

\[ We \quad \text{Weber number } \left( \mu_{\text{g}}^2 d \rho_{\text{g}} / \sigma_{\text{g}} \right) \]

\[ \mu \quad \text{dynamic viscosity} \]

\[ \rho \quad \text{density} \]

\[ \sigma \quad \text{surface tension} \]

**References**


Table 1. VOF versus Experimental Observations

<table>
<thead>
<tr>
<th>Breakup Regimes</th>
<th>Weber Number</th>
<th>$t/t^*$ at Onset</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Present</td>
<td>Dai &amp; Faeth [13]</td>
</tr>
<tr>
<td>Bag breakup</td>
<td>12</td>
<td>13</td>
</tr>
<tr>
<td>Multimode breakup</td>
<td>17</td>
<td>17</td>
</tr>
<tr>
<td>Shear breakup</td>
<td>75</td>
<td>80</td>
</tr>
</tbody>
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Figure 1. Boundary Layer Stripping phenomenological models theorize the stripping of the boundary layer of the drop as the primary reason for the drop breakup a) Left: Schematic of Boundary Layer Stripping model from Chou et al. [4], (b) Right: Typical experimental observations (From “Experimental Investigation of the Aerodynamic Breakup of Liquid Drops” by Wierzba and Takayama [6]; reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.)

Figure 2. Experimental shadowgraph sequence of shock tube experiment from Ranger and Nicholls [1]
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Figure 9. Grid independence check for the 2D axis-symmetric case

Figure 10. (a) Left: Typical observation of drop breakup in (a) Left: bag breakup mode (Reprinted from International Journal of Multiphase Flows, 27, Dai and Faeth, Temporal Properties of Secondary Drop Breakup in the Multimode Breakup Regime, 217-236 Copyright (2001), with permission from Elsevier) (b) Right: shear breakup mode (From “Experimental Investigation of the Aerodynamic Breakup of Liquid Drops” by Wierza and Takayama [6]; reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.)
Figure 11. Bag breakup time sequence from VOF compared with experimental pictures (Reprinted from International Journal of Multiphase Flows, 27, Dai and Faeth, Temporal Properties of Secondary Drop Breakup in the Multimode Breakup Regime, 217-236 Copyright (2001), with permission from Elsevier). Please note that the simulations are a 2D slice through drop, while photographs are not.

Figure 12. Shear breakup time sequence from VOF compared with experimental pictures (Reprinted from International Journal of Multiphase Flows, 27, Dai and Faeth, Temporal Properties of Secondary Drop Breakup in the Multimode Breakup Regime, 217-236 Copyright (2001), with permission from Elsevier)
Figure 13. Comparison of onset of breakup over a range of Weber numbers between VOF and experiments.

Figure 14. Liquid drop breakup as a function of Weber number, Ohnesorge number = 0.0149.
Figure 15. Effect of variation in Reynolds number by changing the drop size at We = 45 for ethanol (a) Top: 600 micron drop diameter, Re = 15, (b) Bottom: 60 micron drop diameter, Re = 4.7

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Figure 20. Time sequence of the shear breakup process using 3D VOF
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Figure 22. 3D VOF of jet in crossflow study to understand jet breakup and near jet, dense spray characteristics