Numerical Simulation of Binary Droplet Collision Using CFD Software Tools

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ABSTRACT

We have computationally investigated the head-on collision between two identical droplets by using commercial software tools based on the volume-of-fluid (VOF) method. The results were compared to that obtained by the front-tracking method and experiments. The simulated collision images were found to agree with the experimental observations only at a low or moderate Weber number (*We*). If *We* became so large that the surfaces were substantially deformed, specifically when the regimes showing separation and breakup were attained, prominent disagreements were generated. In particular, the simulation for phenomena of separation was characterized by exaggeratedly created bubbles near the coalesced interfaces, whereas that for break-up scenario could be affected much by the evaluation of surface curvature and forces as well as the grid construction. Furthermore, the predictions of the transition boundaries between the coalescence and bouncing regimes at lower *We*'s did not exhibit reasonable fidelity. This is because the merging process involves multi-scale physics that cannot be simply resolved by the artificial treatment of the interfaces in the present methodology based only on a macroscopic description of hydrodynamics. This work thus provides examples not suitable for these tools and provokes cautious consideration for those who apply such commercial packages to relevant problems.

Keywords: volume-of-fluid method; front tracking method; droplet collision; coalescence; breakup

1 INTRODUCTION

Numerical simulation has been applied widely to investigate and solve sundry scientific and engineering problems. In this study, we are concerned with the collision dynamics between two droplets, which is a unit element in spraying processes and plays a crucial role in various areas such as meteorology (e.g., rain formation), biological and medical industries, painting and coating techniques, fire fighting, and spray combustion. Among these, the latter is of our particular interest, specifically considering the purposes for modeling and design of related structures like that in liquid-fueled engines. To compute the flow field with different phases constituted of liquids and gases, specific models have been pursued in the near decades, such as VOF method, level set method, and front tracking method. Among the various methodologies, VOF has been used extensively and incorporated into some commercial packages such as CFD-ACE+ and Fluent, which are adopted largely to solve problems with free surfaces accounting for surface tension forces. Due to their amenable and somehow simplified user interfaces, however, it is possible to obtain results that could be incorrectly manipulated and interpreted if the users do not have enough knowledge about the settings and functions. In this report, we intend to clarify certain issues which could be omitted or not noticed when using such software tools. These were presented in our investigation for droplet impacts as reviewed in the following. We do not intend to dig out the problems of the VOF methodology itself, but merely to provide a platform for sharing our experience of using such popular tools with engineers or researchers who may deal with similar problems. In addition, this shall open a perspective for the developers to identify the issues for further improvement and advancement.

The dynamics of binary droplet collision is an essential topic for understanding the physics of drop impact. For the limiting situation of head-on collision, recent studies [1,2] showed four typical regimes of distinctively different outcomes with variation of the collision Weber number, $We = \rho_\ell V_r^2 D/\sigma$, where D is the droplet radius, V_r the relative velocity of the droplets, and ρ_ℓ and σ respectively the density and surface tension of the liquid. With increase of *We*, these four regimes are categorized according to: (I) permanent coalescence after minor droplet deformation, (II) bouncing, (III) permanent coalescence after substantial droplet deformation, and (IV) coalescence followed by separation and concomitant production of daughter droplets.

The transition between regimes III and IV has been successfully described in Ref. [2] by assessing whether the kinetic energy of the impact, plus the surface energy of the impacting droplets, can be adequately dissipated through the internal motion generated during the collision, such that the remaining energy is just sufficient to constitute the surface energy of the spheroidized merged mass. The last regime, i.e., of separation, has been studied broadly, whose dynamics is typically governed by the hydrodynamics, and the onset of the transitional boundary can be estimated via the conservation of energy. Consequently, the events can be simulated essentially based on the global motions of the interfaces in the framework of continuum mechanics. The transitions between regimes I and II, and between regimes II and III, however, cannot be directly computed because the occurrences depend on the competing of repulsive pressure between the approaching interfaces and impact inertia which involves complex structures dominating at

different scales such as short-range intermolecular forces and mesoscale effects of gas rarefaction [3]. This difficulty thus has been impeding numerical studies for such critical transformations. Notwithstanding, computations in terms of a coupling with the experimental results were recently conducted by Pan *et al*. [3] based on a front tracking method.

Recognizing the power provided by the numerical tools, researchers and engineers have been adopting commercial packages to simulate relevant problems. Almost all of the successful studies using commercialized CFD programs were performed in situations where the geometry did not involve intensive deformation and interactions of the interfaces and the flows were usually associated with low *We* or *Re*. The present study was motivated by our intention to apply commercial software, based on VOF, for simulation of the collision dynamics and to compare the results with our experimental observations, particularly for those found recently in [4] with substantially large *We* and *Re*. This shall provide a deeper insight to the underlying mechanism and help develop theoretical modeling and predictions. With substantial effort, however, it was found that such popular commercial codes did actually have their own constraints in simulating such flows with complex interactions of moving interfaces, although they had been applied widely to simple multiphase flows with free surfaces [5-7].

2 NUMERICAL AND EXPERIMENTAL SPECIFICATIONS

We have adopted the software tools of Fluent and CFD-ACE+ for simulations of binary droplet collision. The results are compared with that obtained by the experiments and the front tracking method. Details of the latter approaches should be referred to our previous studies [3,4] while the former can be directed to a great number of references in the literature based on VOF method [8-10] as well as our comprehensive report that is to be submitted [11].

3 RESULTS AND DISCUSSION

We have tested the simulation in terms of Fluent but the evolution was not successfully simulated, in particular when the Weber number became moderately high. The impact consequence always led to coalescence even in the nominal regime of bouncing at a low Weber number. The following discussion is based on the simulation in terms of CFD-ACE+.

3.1 Droplet collision at low Weber number

Figures 1 and 2 show the experimentally obtained [3] and computed droplet collision sequences that illustrate the transition from soft coalescence to bouncing with increasing Weber number. When the sequence was initially computed by CFD-ACE+, the simulation results were close to that of Fluent showing persistent merging at low *We* or earlier rupturing at moderate/high *We*. If the specific option of "surface-tension force damping" was turned on, however, agreement with the experimental results was substantially enhanced. As shown in Figure 1, the approaching interfaces are impeded, which are not merged immediately (in contrast to that presented by Fluent), due to the intervening gas film [2,3], and deformed substantially before merging. The interfaces are then coalesced at an instant close to the experimentally recorded time. The following evolution consequently exhibits a consensus with the experiment. Nonetheless, because of such an artificial simulation of merging that is based on the numerical model, some disagreement is inevitably created. Specifically, as compared to that of front-tracking method in which the rupture of the interfaces is adjusted according to the experimental observation (and so a strong dependence on the modeling is excluded), the evolution phase is less satisfactorily reproduced (ostensible at the later stages).

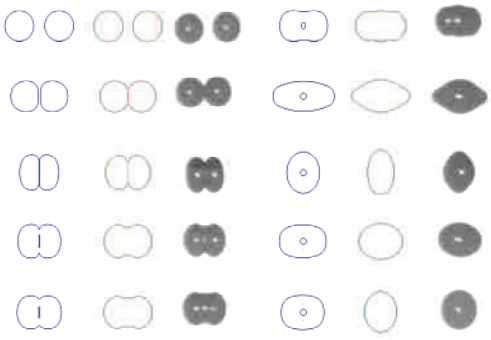

Figure 1: Comparison of CFD-ACE+ simulation (left column) with front-tracking simulation (central column) and experiments published in [3] (right column) for coalescence near the boundary between regimes I and II.

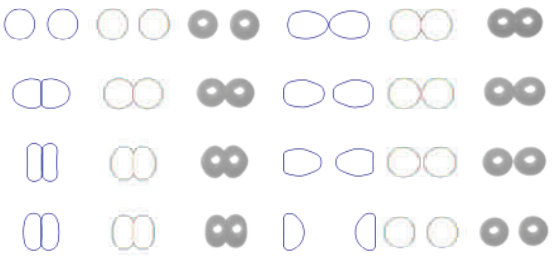

Figure 2: Comparison of CFD-ACE+ simulation (left column) with front-tracking simulation (central column) and experiments published in [3] (right column) for bouncing near the boundary between regimes I and II.

An intriguing phenomenon observed is the creation of a bubble in the central region after the merging of interfaces. More bubbles are even generated (above and below the central one) at a later time. The accuracy of producing such

phenomena will be discussed with more elaborated conditions.

3.2 Effect of surface-tension force damping

As mentioned in the manual, the function of surface-tension force damping (or capillary-wave damping) equipped in CFD-ACE+ is to locally increase the viscosity in the vicinity of the interface. It thereby reduces the tangential velocities and damps the capillary waves that are invariably generated at the interface under surface-tension forces. These waves are of no interest particularly for the problems in which only the gross propagation of the interface is being considered. This may enable larger time steps for sufficient convergence which is controlled by the CFL number. This function would be particularly useful in the present problems of interfaces associated with rapid changes, large curvatures, and/or strong surface-tension forces, thus leading to closer agreement with the experimental results at least during the early times.

The default magnification of the viscosity is set to 500 times increase in the gas phase near the interface and 10 times larger in the liquid phase. It was found, however, that bouncing could not be created near the transition boundary (regime I to II) unless the increase in local viscosity of the gas was larger, say, by 600 times. The result is demonstrated in Figure 2. It is seen that, although the interfaces are kept separated and simulated moderately well at the early stage, the later contours of deformation are ostensibly distorted. To be noted in particular, since the droplets are elongated erroneously after bouncing off and the computational domain is the same as that of front tracking approach, they touch the side walls more quickly. Therefore the droplets are "flattened" by the walls at later times.

3.3 Formation of bubbles and removal of flotsam and jetsam

The formation of bubbles is questionable regarding the accuracy of the numerical models. CFD-ACE+ is built with a function of "removal of flotsam and jetsam," which is not incorporated in Fluent. One of the known defects of VOF method is the creation of small isolated droplets of liquid in gas regions, and of small isolated bubbles of gas in liquid regions [5]. This function is to remove the bubbles that would be artificially generated or at least prevent some of the negative effects before the "flotsam and jetsam" begin to affect the solution.

After this option was turned on, it indeed suppressed the small bubbles that could otherwise be formed during the collision [11]. However, a primary bubble, which could be related to the trapped gas in between the interfaces, is clearly generated in the simulated sequences as shown. Even if we have largely increased the grid resolution, a bubble is always established at the center. These figures demonstrate the same consequence of bubble formation in terms of different mesh structures in CFD-ACE+ and Fluent by structured (rectangular) and unstructured (triangular) cells, respectively. The scale of the bubble does not vary much even if it is filled with more cells.

3.4 Droplet collision at moderate/high Weber number

When *We* is sufficiently large, the droplets coalesce temporarily and then separate. The simulation via CFD-ACE+ is essentially consistent with the experimental sequence, whereas the phase is shifted slightly. If *We* is further increased, a satellite droplet is formed by the initial ligament connecting the two primary droplets after the separation. While the qualitative evolution is close to that of experiment, the quantities such as separation distance of the droplets and the size of the satellite droplet are different.

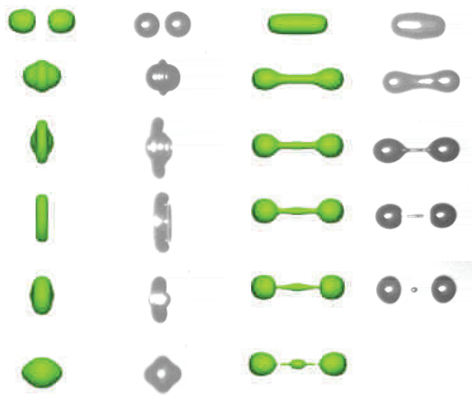

Figure 3: CFD-ACE+ simulation compared with the experimental results, showing separation followed by a satellite droplet.

Such a discrepancy can be identified in Figure 3, where the experimental pictures were obtained with high spatial resolution using a synchronization technique. It is seen that, not only the breaking phase of the satellite droplet (and the diameter of the ligament) differs, but its final size also appears much larger than the real one. Taking a projection view into the droplets, as shown in Figure 4, we find that there is a huge bubble formed inside the satellite droplet. Furthermore, quite a few small bubbles are created after the impact, which travel inside the droplet and may coalesce with others. Due to the exaggeratedly magnified size, therefore, the satellite droplet cannot approach the observed size of real cases. It demonstrates the falsified formation of bubbles.

Formation of bubbles has also been discussed in previous studies. Because of the gas film trapped between the approaching interfaces, bubbles could indeed occur in the collision [3,12,13]. Accurate simulations for such bubbles and their evolutions, however, are particularly difficult in the present problems where the coalesced droplets are further elongated and thus leads to a thin ligament inside which a big bubble is formed (Figure 4);

thereby the thin layer (or the "skin") between the inside and the outside gas media requires substantial grid points to prevent unexpected rupture. Furthermore, due to accumulated errors of computation caused by the time integration or interpolation of the field properties such as velocity, the mass of gas part could deviate gradually from the original condition. As a consequence, the merged droplets may readily rupture after creation of artificial bubbles, thus leading to falsified evolution if more errors are accumulated without adequate treatment immediately.

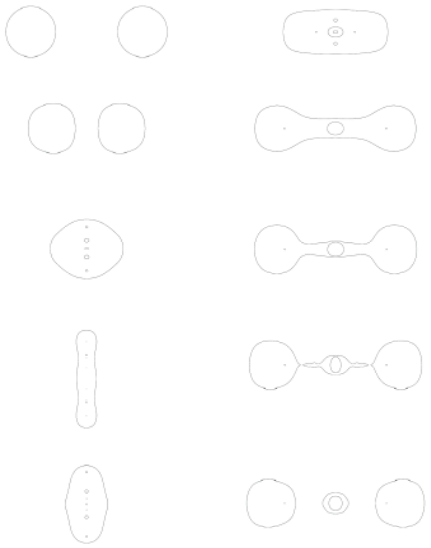

Figure 4: Transient images of bubble formation.

3.5 Simulated collision events at high Weber number

While the evolution of binary droplet collision at moderate or low Weber numbers has been studied broadly, that at high *We* was only recently investigated in a systematical way by Pan *et al*. [4]. Specific phenomena are simulated and will be discussed in [11] for the formation of fingers at the rim of an expanding/retracting disk and splattering of multiple secondary droplets.

4 CONCLUSIONS

In this study, we have evaluated the applicability of numerical simulation for binary droplet collision using the volume-of-fluid method that is embedded in the commercial codes of CFD-ACE+ and Fluent. The computed results were compared to that obtained by experiments and the front-tracking method, for the regimes of coalescence and bouncing at low/moderate Weber numbers. It was shown that, unlike the latter approach which always kept the interface and density stratification sharp, VOF needed to reconstruct the interface and automatically led to merging. The outcome might not be quantitatively coincident with the experimental measurement of transition boundaries between coalescence and bouncing because the strategy did not account for the mesoscopic physics, such as compressibility and rarefied gas effects, and microscopic mechanisms, such as intermolecular forces. These results were purely yielded by numerics based on hydrodynamics. Such a difficulty in connecting the disparate scales was avoided by manually setting the merging instant of the approaching interfaces in the front-tracking simulation, according to the experimental observations.

As shown by the computations for the regimes at higher *We*'s, e.g., coalescence followed by separation and satellite droplets, bubbles were inaccurately created. In particular, this can be demonstrated by a much larger size of the satellite droplet as compared to the experimentally observed size. It was caused by a tremendous bubble generated artificially during the simulated collision, which obviously misled the result. From these falsified consequences of automatic merging of liquid surfaces and growth of bubbles, we conjecture that the phases of these fluids might have been misinterpreted, specifically near the interfaces, by the tested numerical tools. Furthermore, Fluent VOF did not incorporate the function of surface force damping that was implemented in CFD-ACE+; this was found to be a crucial mechanism for properly simulating the interactions of approaching interfaces with rapid motions and significant contour variations.

ACKNOWLEDGMENTS

The work was supported by NSC projects: 97-2221-E-002-215 and 98-2221-E-002-122-MY2. We are grateful to NCHC for computer time and facilities.

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