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# High fidelity simulations of binary collisions of liquid drops

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**Abstract**

The phenomena of binary droplet collision is seen in dispersed phase systems such as sprays in internal combustion engines, gas turbines, etc. The present work aims at understanding off-center collision dynamics of two droplets of unequal sizes. High fidelity simulations are performed using three dimensional, two phase- finite volume based solver in OpenFOAM platform. Volume of fluid (VOF) method is used for interface capturing. Navier-Stokes equations are solved using a projection algorithm. Simulations are done with MPI parallelization to meet the computational demand. The solver is validated against droplet splashing benchmark test case. The present numerical results study the effect of impact parameter and diameter ratio on droplet collision dynamics.

**Keywords**: droplet collision, two-phase flow, Volume of fluid method

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## Introduction

Numerical studies on droplet collision remain a research topic of great interest due to its significance mainly in dense spray systems such as internal combustion engines, gas turbines etc. Liquid drop collisions can be studied with physical experimentation, modeling and numerical simulations. Experimental studies can be found in the literature, in which motion of droplets are inferred to propose empirical correlations for drag and lift forces acting on particles [1, 2]. Many experimental investigations [3, 4, 5] have been performed to develop a monogram representing different regimes occurring after binary droplet collision. Ashgriz and Poo [3] had an extensive experimental investigation of binary collision of water drops for different combinations of diameter ratios and impact parameters in the Weber number range 1 to 100. Ashgriz and Poo [3] and Estrade et al. [5] also developed theoretical models to predict the outcome of collision regimes and compared with experimental results. Jiang et al. [4] studied collision dynamics of water droplets and normal-alkane droplets. For head-on collisions of water droplets they reported permanent coalescence for all cases. But during fuel droplet collisions, they have identified five different regimes , which can be summarized as:

1. Coalescence with minor deformation
2. Bouncing after substantial deformation
3. Coalescence with substantial deformation
4. Coalescence followed by splitting
5. Grazing collision

The first four regimes are observed for both head-on and off-centre collisions. The fifth regime is for off-centre collisions only. This regime involves high energy collisions. Satellite droplets are usually produced in regimes 4 and 5. The quantities which influence the output collision regime are droplet relative velocity, density and viscosity of fluids, Weber number, impact parameter and ratio of droplet diameters. Generally impact parameter is defined as the ratio of the projection of the droplet centre-to-centre line on-to the direction normal to the relative droplet velocity to the average droplet diameter. The limitation with experimental studies is that the physical processes at the interface often occurs at very small time and length scales, which cannot be captured well by conventional experimental apparatus. Numerical simulations have gained importance because of its ability to resolve the small scale flow physics in interfacial multiphase flow physics [6]. Additionally numerical simulations aid in studying the effect of a particular parameter among the large number of parameters involved in the collision process. Model inputs required for atomization spray models and droplet transport can be derived from direct numerical simulations or physical experiments. In the present investigation, numerical simulations are performed to study binary droplet collision. Recent numerical studies of droplet collision are briefly presented here.

Numerical simulations in multiphase flows are generally carried out using front tracking methods [7] or front capturing methods [8, 9]. But front tracking methods are not well adapted to describe flows involving large interface deformation like droplet collision studies. Front capturing methods were successful in simulating flows with large deformation and breakup. Two main approaches in front capturing methods are volume of fluid (VOF) [8] and level-set (LS) [9] methods. Nobari et al. [12] simulated head-on collision of equal sized droplets using front tracking method with axi-symmetric formulation. They predicted different regimes of equal sized droplet collisions by artificially modelling layer at the interface rupture. Later Nobari and Tryggvason [13] extended the methodology to simulate 3-D simulations of off-centre binary collisions of equal sized droplets. The reported simulations are limited to low Reynolds number and Weber number. Poo and Ashgriz [14] studied collision dynamics of 2-D binary droplets using VOF method. The obtained results were different from the 3-D results due to surface tension effect. Nikolopoulos et al. [15] studied 3-D off-centre collision dynamics of hydrocarbon droplets at various Weber and Reynolds numbers. Their numerical method employs VOF method based on high resolution differencing scheme called CICSAM [16]. The effect of Weber number and impact parameter on the main characteristics of ligament was studied. Graham et al. [17] have reported both experimental and numerical study of coalescence of a falling water droplet with a sessile water droplet on a solid surface. They have performed numerical simulations with VOF method in OpenFOAM cfd framework. This VOF methodology is formulated based on a bounded compressive scheme [18]. They have obtained good agreement between experimental and numerical results.

Pan and Suga [19] reported a remarkable work on binary liquid droplet collision using level set method. Their Navier-Stokes based simulations were able to capture bouncing collision regime but unable to capture secondary coalescence collision (coalescence after minor deformation at lower Weber numbers). They proposed that this mechanism is dominated by intermolecular forces, which cannot be captured by a macroscopic numerical model. They also studied the mechanism of satellite droplet formation in head-on and off-centre collisions. To the knowledge of the authors, studies on numerical simulations with off-centre binary collisions of unequal sized droplets are rare. In this paper, a numerical investigation of binary collision of two unequal sized droplets in a liquid gas system with a high density ratio is presented using VOF methodology.

## Governing equations and methodology

The flow considered is assumed to be three-dimensional, incompressible, variable density, iso-thermal and immiscible. The governing mass and momentum conservation equations can be written in vector form as:

$$\nabla.U = 0 \tag{1}$$

$$\rho(\frac{\partial U}{\partial t} + U.\nabla U) = -\nabla p + \nabla.(\mu \nabla U) + F \tag{2}$$

To capture the interface between the gas and liquid, an additional equation is solved

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (U\alpha) = 0 \tag{3}$$

The term $F$ in equation 2 represents the body force term which include the force due to surface tension. The variable $\alpha$

in equation 4 stands for volume fraction of fluid, defined as the fraction of the volume that the reference fluid occupies in a given computational cell. Equation 4 is solved using VOF methodology. All the simulations are done using OpenFOAM CFD framework. OpenFOAM uses compressive scheme [18, 20] for the discretization of the volume fraction equation. This scheme adds a compressive term to the advection equation as shown in equation 4.

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha U) + \nabla \cdot (\alpha \beta U_c) = 0 \tag{4}$$

where $\beta = 1 - \alpha$ and $U_c = U_l - U_g$ is the compressive velocity. The last term in left hand side of equation 4 is called artificial compression term and is active only at the interface.The volume fraction is advected using Multi- dimensional Universal Limiter with Explicit Solution (MULES) which is based on flux corrected transport [21, 22] to give a bounded solution. Algorithm followed in the OpenFOAM's standard multiphase flow solver *interfoam* can be obtained at [23]. In the current work standard explicit algorithm namely SMAC (Simplified Marker and Cell) was implemented in OpenFOAM platform to solve the Navier-Stokes equations. The implementation of explicit algorithm has resulted in lesser computational time when compared to other implicit algorithms in OpenFOAM.

**Validation**

The present solver is validated against a droplet splashing benchmark test case. The test case is briefly presented here.

A cuboidal domain is considered with liquid filled to a certain height, so as to form a thin liquid sheet. A water droplet initially at a certain height above the liquid film surface is allowed to fall with a finite initial velocity, under the action of gravitational force ($g = 9.81 m/s^2$). Present validation is done based on the experimental study reported by Cossali et al. [24]. Physical parameters used in the simulation are presented in Table 1. A cuboidal domain of size $6.5d \times 1.75d \times 6.5d$ is considered. Initial droplet diameter is covered by 50 computational cells which has resulted in a total mesh size of $260 \times 70 \times 260$. As the droplet hits the water film, a crater is formed which grows in diameter with respect to time. Impact of droplet splashing at different time instants obtained from simulation is shown in Fig. 1. The non-dimensional crater diameter is plotted against non-dimensional time and the results are compared with those of Cossali et al. [24]. Non dimensional crater diameter is defined as the ratio of crown diameter to initial drop diameter. A near match is obtained between the present solver and the experiment, as shown in Fig. 2. These results shows that the present solver in OpenFOAM is able to simulate high density ratio and high viscosity ratio flows.

**Results and discussions**

Collision of two unequal sized liquid droplets is considered. The computational domain is shown in Fig. 3 . Among the different parameters influencing droplet collision, effect of impact parameter and droplet diameter ratio are studied. Depending on these parameters, the outcome of the collision is observed to be coalescence or stretching separation with or without formation of satellite droplets. A collision occurs only when $0 < x < 1$. The physical properties of the fluids used in the simulations are given in Table 2. Diameter of the smaller droplet is kept constant throughout and is equal to 100 $\mu$m. The smaller droplet diameter is covered by 50 cells. At the beginning of the simulation ($t = 0$), each droplet is given an initial velocity of 0.5 $m/s$ in opposite direction. This gives Reynolds number and Weber number both equal to 100. Here the smaller droplet diameter is taken as the characteristic length. Initially, the droplets are separated by a distance of 4 grid cells in the direction of relative velocity (along x-direction). In order to capture the liquid within the computational domain, the size of the domain is extended based on impact parameter or droplet diameter. Accordingly the mesh size was in the range 3.1 to 7.5 million uniform cells for the cases considered. Although this mesh count may not completely resolve the tiny satellite droplet, it is expected to capture the features of the droplet motion and ligament formation during stretching. For boundary conditions, gradient of the normal velocity is given as zero on all boundaries. Also zero pressure gradient is imposed on all boundaries except at the top face. For the top face pressure is given as zero.

**Effect of impact parameter**

Four different cases were studied with impact parameter $x$= 0, 0.25, 0.5 and 0.75. Impact parameter of zero implies head on collision of droplets. Diameter ratio equal to 1.5 is used for all the four cases. Time evolution of volume fraction contours during droplet collision for these cases are shown in Fig. 4. For $x$=0 case, after collision the larger droplets absorbs the impact of the smaller droplet and continues to move together in the direction of initial velocity of larger droplet. This can be expected due to the greater inertial force of the larger droplet. It is observed that the smaller droplet merges with the larger droplet and leading to lateral expansion of the liquid blob. This liquid structure appears like a disc (shown at $t$= 0.5 $ms$ in Fig. 4 (a)). This development of disc is a result of higher stagnation pressure than surface tension pressure. In the later stages, surface tension pressure exceeds the stagnation pressure resulting in contraction of disc which takes a distorted shape finally as shown in Fig. 4 (a) at 1.25 ms. At the end of the simulation the liquid remains coalesced with substantial deformation.

For the case with $x$= 0.25, a slight offset is present between the droplets. Due to the non-zero impact parameter, the region of interaction between larger and smaller droplet decreases when compared to head-on collision. Initially the smaller droplet merges in to the larger droplet as shown in Fig. 4 (b) at $t$=0.125 $ms$. Similar to the head-on collision case, coalesced droplet elongates to a disc shaped structure. One of the primary difference between a head-on collision and off-center collision is that, in addition to the translational motion, coalesced droplet is also associated with rotational motion. Due to the rotational motion, the coalesced drop is now at an oblique angle as shown in Fig. 4 (b) at $t$= 0.625 $ms$. For the case of off-center collision of equal sized droplets reported in [19, 15], center of rotation appears to be at equal distance from the two droplet centers. But in the present case of unequal sized droplets, center of rotation is closer towards the smaller droplet center. This is evidenced by the location of thinned region between the bulbous

ends being nearer to smaller bulged structure. At the end of the simulation the droplet remains coalesced with a distorted shape, this implies that the kinetic energy of the internal flow is still not sufficient enough to overcome the surface energy. The combined drop oscillates until a spherical drop is formed.

The next case is considered with $x$= 0.5. As the impact parameter is significant only a portion of the droplets will come in to direct contact and the remaining portions of the drops tend to continue in the direction of their initial velocity. This results in the stretching of the region of interaction. Initially coalesced droplet elongates in to a disc shaped structure and continue to move under the influence of both translational and rotational forces. At later stage, at $t$= 1.925 *ms*, as shown in figure 4 (c), the two liquid blobs move apart with the formation of a bridge in-between. This stretched ligament breaks down at an instant when stretching energy dominates the surface energy, this is referred as end-pinching effect [19]. The separated liquid drops can be seen at $t$= 2 *ms* in Fig. 4 (c). The determination of the critical impact parameter for this transition from coalescence with substantial deformation to stretching separation requires further simulations.

The final case in this section is with $x$= 0.75. For this high impact parameter case, stretching separation is more likely to occur as the momentum of the smaller droplet is much less than the inertia and surface forces in the region of interaction. Similar to $x$= 0.5 case, the liquid blobs in the coalesced structure move apart with a bridge in-between. But this connecting bridge is now very thin because of lesser region of droplet interaction. Capillary waves can be observed on this ligament as shown in Figure 4 (d) at $t$= 1.775 *ms*. It is believed that this thin liquid ligament breaks up due to capillary instability into satellite droplets. This ligament can breakup into a single droplet or multiple droplets depending on the impact parameter. For the present case multiple satellite droplets are formed as shown in Fig. 4 (d) at $t$= 1.975 *ms*. This phenomena of ligament breakup due to capillary wave instability is previously reported by Pan and Suga [19] in their simulations for a case with approximately similar parameters. An image comparing the satellite droplet formation between present simulation and Pan and Suga [19] is shown in Fig. 5. Short wavelength waves on ligaments (expected due to capillary instability) can be observed in the figure in both the cases.

**Effect of diameter ratio**

Four different cases were studied with larger droplet to smaller droplet diameter ratio $\Delta$= 1, 1.25, 1.5 and 1.75. All the cases were simulated with a fixed impact parameter equal to 0.5. The evolution of droplets during collision for cases $\Delta$=1, 1.25 and 1.75 is shown in Fig. 6 (a), Fig. 6(b) and Fig. 6(c) respectively. The case with $\Delta$= 1.5 is same as the previous case with $x$=0.5 (Figure 4 (c)).

The diameter ratio one corresponds to the collision of equal sized droplets. As the diameter ratio increases, the interaction region for the droplets increases. Simulations have shown the cases $\Delta$= 1 and 1.25 in the stretching separation collision regime. Because of the less interaction region and high Weber number, one can predict the possibility of end pinching and breakup for these cases. The initial processes like merging, lateral expansion of the liquid can be observed from the Figure 6 (a) at time $t$= 0.2 ms. In the later stages, the two liquid blobs move apart with a connecting bridge in-between. As mentioned before, this stretched ligament breaks down at an instant when stretching energy dominates the surface energy. This pinched off ligament has further broke down into satellite droplets due to the action of surface tension. It was mentioned in Ashgriz and Poo [3] that the collision outcome of two unequal-size drops is governed by two opposing effects, namely drop drainage and drop stretching. Drop drainage is the flow of liquid from high pressure drop to the interaction region to form a liquid bridge. With the increase in impact parameter, stretching effect increases and shorter will be the time for drainage. These two opposing effects determine the size of the satellite droplets. The current case with $\Delta$ =1 can be qualitatively compared with an experimental case reported by Ashgriz and Poo [3]. Fig. 7 shows the comparison of present simulation with Ashgriz and Poo [3].It can be seen from the figure that two satellite droplets are formed in both the cases, which shows that the current simulations can qualitatively predict the droplet separation regimes.

The case $\Delta$= 1.5 is same as the previous $x$= 0.5 case. As seen before, this case falls under stretching separation regime but with no satellite drop formation.

The last case is with $\Delta$= 1.75. Due to the high diameter ratio, the mass in the small drop will have high tendency to flow in to the large drop. After the initial impact, the small drop forms a cavity in the large drop. This coalesced structure elongates in lateral direction and continues to flow under translational and rotational forces. This coalesced droplet contracts radially inward as a result of the surface tension forces. Similar to the $x$=0.25 case, the droplet remains coalesced with a distorted shape, which means that surface energy is dominating the internal kinetic energy of the droplet. So this regime can be called as coalescence with substatntial deformation.

**Conclusion**

Numerical investigation was done to describe the off-centre binary droplet collision dynamics. 3-D simulations were performed and VOF methodology is used for interface capturing. The effect of impact parameter and droplet diameter ratio is studied. Time evolution of the droplet structures during collision is well captured. Two collision regimes were observed during present off-centre collision simulations namely, coalescence and stretching separation. The stretching separation regime can be with or without formation of satellite droplets. For a given Weber number, droplet collision regime changes from coalescence to stretching separation as the impact parameter increases. The determination of the critical value for this transition requires further simulations. In the stretching separation regime, increase in impact parameter has resulted in formation of satellite droplets. Formation of satellite droplets at moderate impact parameter is observed to be due to end-pinching effect while at high impact parameter it is observed to be due to capillary wave instability of the liquid ligament. For a given impact parameter if the ratio

of lager droplet to smaller droplet increases, droplets are more prone to coalescence.

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| Fluid | Drop diameter (d) $(m)$ | Height of liquid film $(m)$ | Drop impact velocity $(m/s)$ | Density $(Kg/m^3)$ | Viscosity $(Kg/ms)$ | Surface tension $(N/m)$ |
|---|---|---|---|---|---|---|
| Liquid | 5.1e-3 | 5e-4 | 2.14 | 1000 | 1e-3 | 7.3e-2 |
| Gas | | | | 1 | 2e-5 | |

**Table 1.** Physical parameters used in droplet splashing simulation.

| Fluid | Density $(Kg/m^3)$ | Viscosity $(Kg/ms)$ | Surface tension $(N/m)$ |
|---|---|---|---|
| Liquid | 1000 | 1e-3 | 1e-3 |
| Gas | 1 | 2e-5 | |

**Table 2.** Physical properties of fluids in collision cases.

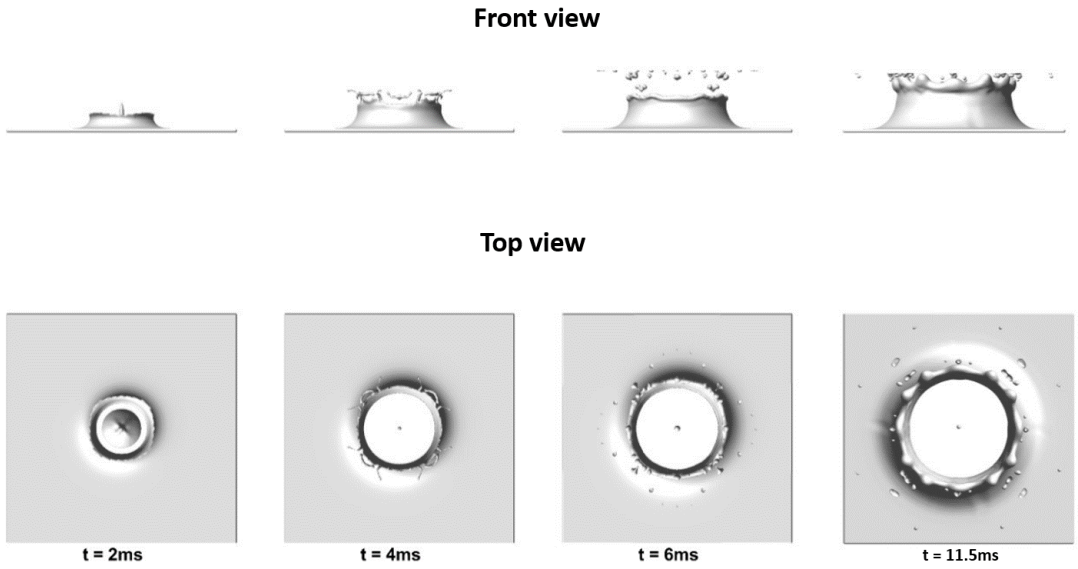


**Figure 1.** Droplet splashing at different time instants.

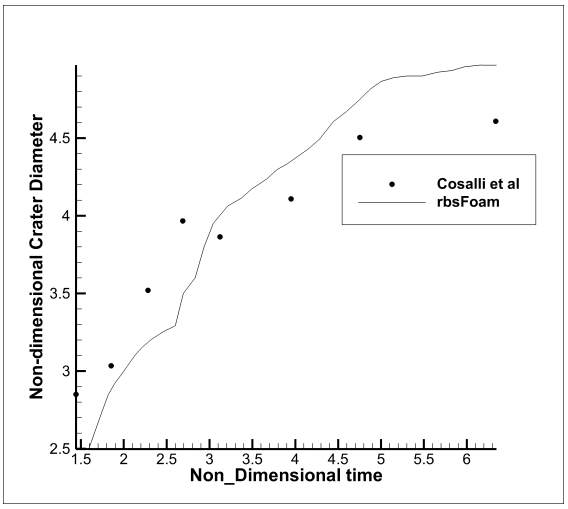


**Figure 2.** Comparison of present simulation (rbsFoam) with experiment [24].

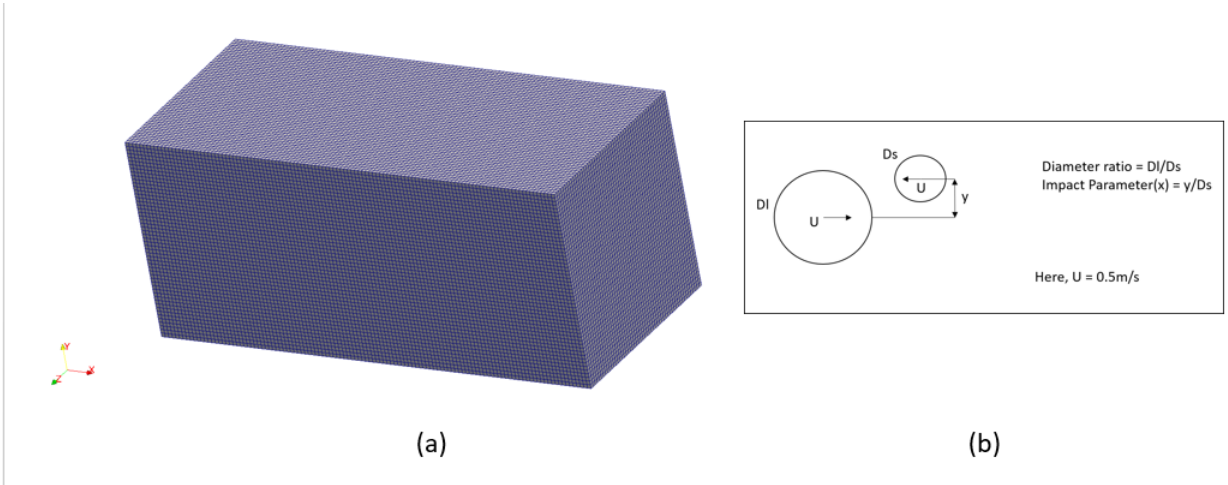


**Figure 3.** Illustration of computational domain.

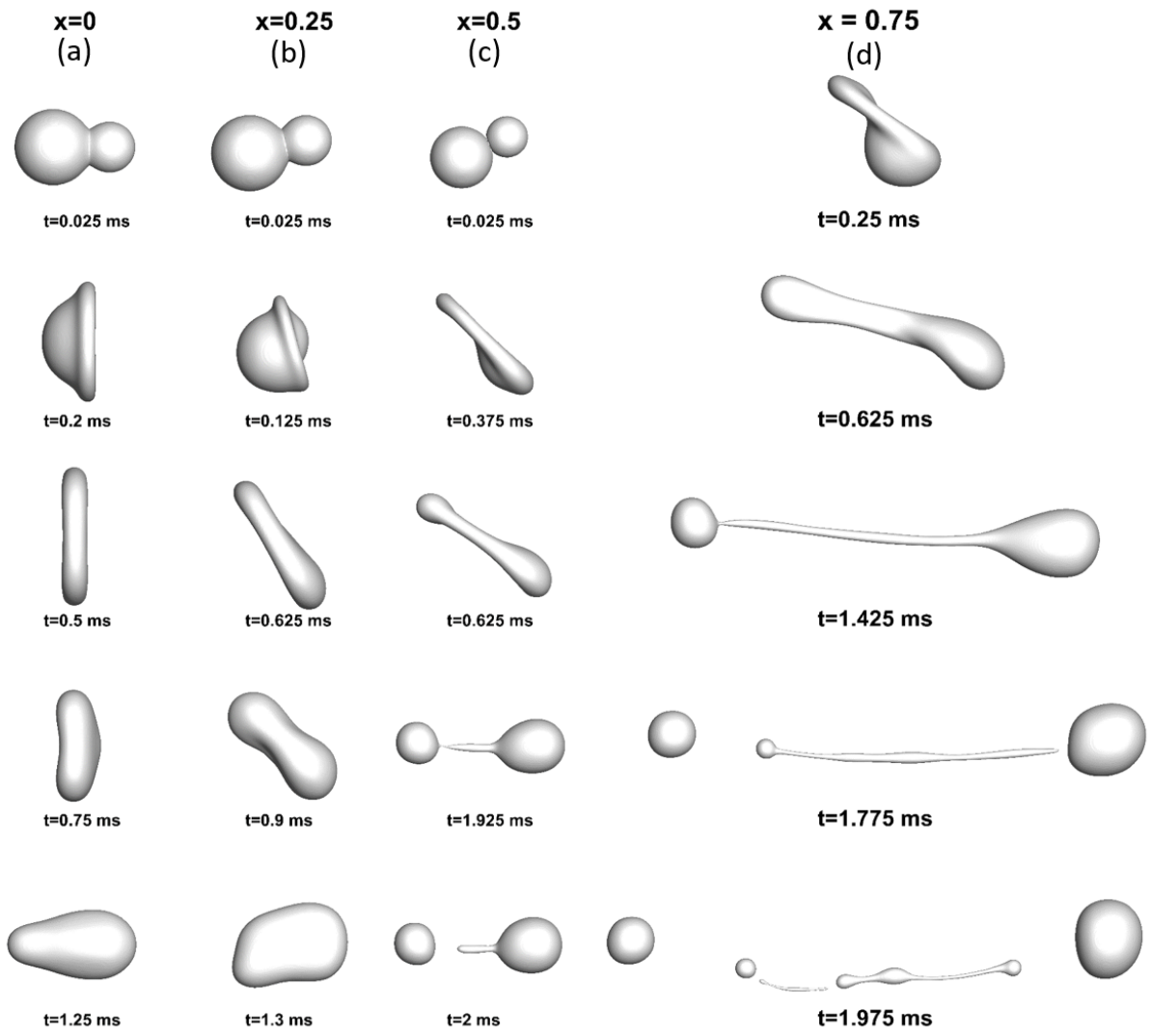


**Figure 4.** Time evolution of droplets for cases $x$=0, 0.25, 0.5, 0.75.

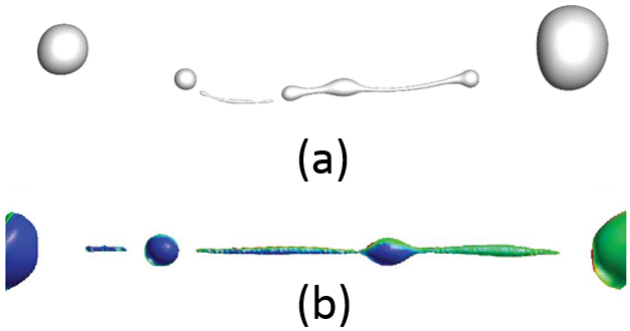


**Figure 5.** Disintegration of ligaments in to satellite drops (due to capillary wave instability). (a) Present simulation, $x$=0.75, We= 100 (b) Pan and Suga [19], $x = 0.7$, We= 165.

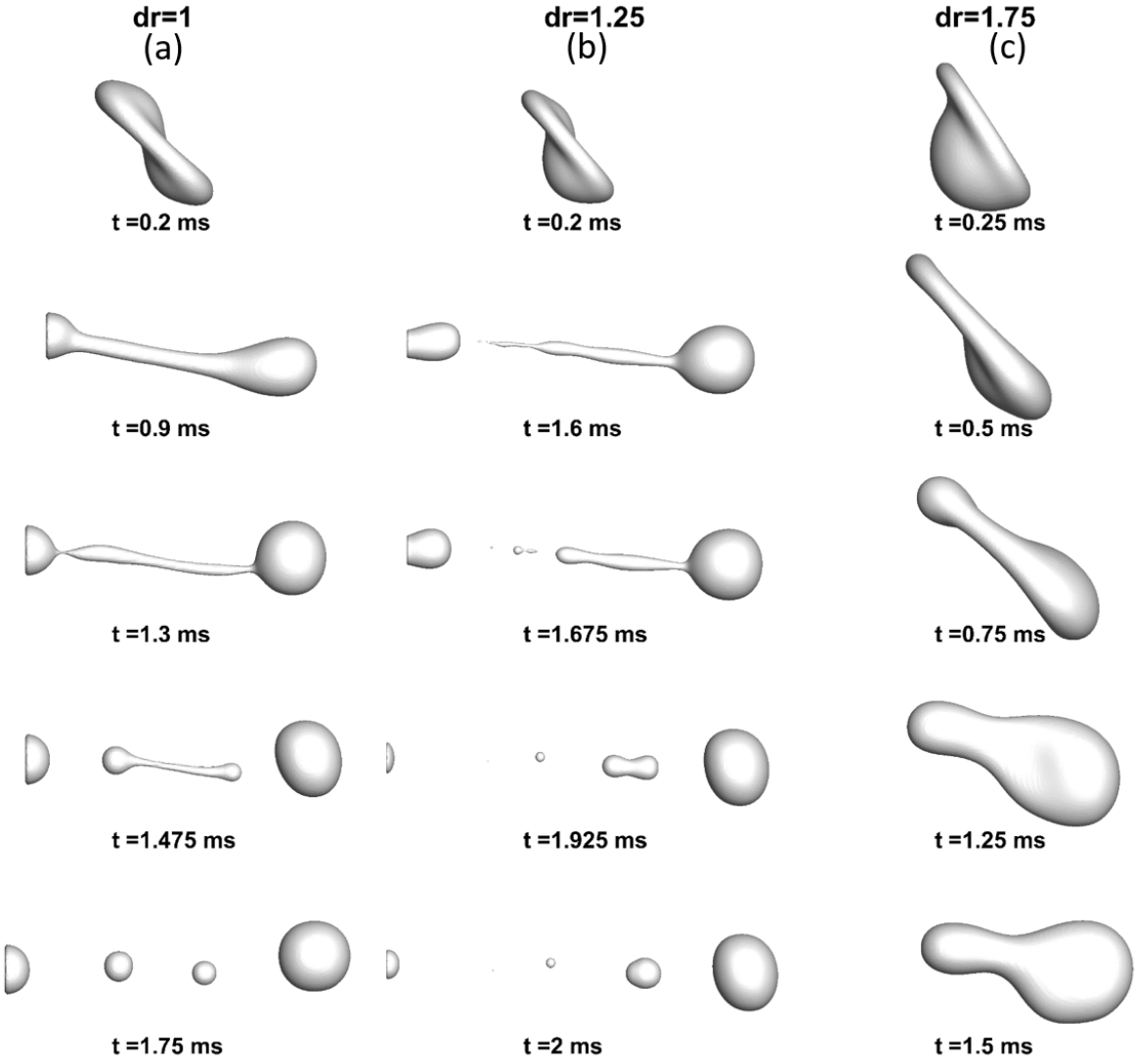


**Figure 6.** Collision process for cases Δ= 1, 1.25 and 1.75.

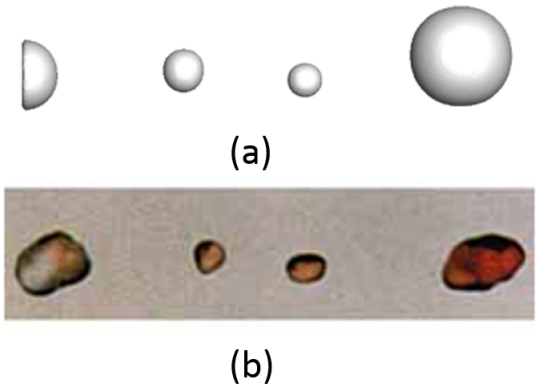


**Figure 7.** Stretching separation at Δ= 1 (a) Present simulation *We*=100, *x*=0.5 (b) Ashgriz and Poo [3] *We*=83, *x*=0.43.