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Collision-induced jet-like mixing for droplets of unequal-sizes

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ABSTRACT

The internal mixing of droplets upon coalescence is of fundamental importance to a number of applications in microfluidics, micro-scale heat and mass transfer, and rocket engine propulsion. Compared to the well-known surface-tension-induced jet-like mixing in the coalescence of inertialess droplets, collision-induced jet-like mixing was observed recently and remains inadequately understood. In the present study, the collision dynamics and internal mixing of droplets of unequal sizes was numerical simulated by using the lattice Boltzmann phase-field method, with emphasis on unraveling the mechanism of the internal jet formation and therefore on exploring strategies to facilitate such a mixing pattern. The results show that the formation of the internal jet requires two synergetic flow motions favoring low *Oh* number and high *We* number: the capillary-pressure-driven radial converging flow induced by the crater restoration to detach the spreading smaller droplet from the surface, and the impact-inertia-driven axial motion along the crater surface to drive the penetration of the detached fluid. The jet-like structure was found to correlate with the evolution of a main vortex ring, which is formed by the vorticity generation on the interface during initial impact, and transported into the droplet during subsequent oscillations. However, due to the absence of the bulge retraction that generates a significant amount of vorticity and to the extended duration for the jet formation, the main vortex is much less intensive compared to that formed by the inertialess droplet coalescence and is therefore less capable of inducing obvious vortex-ring structure in the mixing pattern. Further simulations by manipulating the disparity of the droplet sizes and the disparity of the liquid viscosities show that, the collision of a larger droplet with lower viscosity with a smaller droplet with higher viscosity is effective in facilitating jet-like mixing.

1. Introduction

Droplet collision in a gaseous environment is of fundamental relevance to many natural and industrial processes such as rain/-cloud formation, ink-jet printing, spray coating, and spray combustion in engines. For decades, great efforts including experimental [1–6], numerical [7–12], and theoretical investigations [13], have been devoted to unravel the rich phenomena and the multi-scale physics, with emphasis on identifying collision outcomes and their dependence on the collision parameters. It has been well recognized that the colliding droplets, with increasing impact inertia, can lead to the nonmonotonic outcomes of "permanent coalescence with minor deformation" – "bouncing" – "permanent coalescence with large deformation" – "separation subsequent to temporary coalescence", with the coalescence/bouncing transition depending on whether or not the gas film could be sufficiently drained out, and the coalescence/separation transition depending on whether or not the excessive kinetic energy could be held by surface tension.

Recently, there is increasing interest in the internal mixing within the merged droplet, especially for its potential in the applications such as property design in microfluidics [14,15], rocket engine ignition utilizing gelled hypergolic propellants (GHP) [16], and color manipulation in ink-jet printing [17,18]. Take the propulsion systems utilizing GHP for instance, since the fuel and the oxidizer are sprayed separately into the combustion chamber, while their vapor pressure are too low to form flammable gaseous mixture due to gelation, ignition could be only triggered by the liquid-phase reactions in the merged droplet containing both fuel and oxidizer liquid mass. Therefore, unraveling and facilitating efficient mixing is critical to the viability of utilizing GHP.

It is noted that the mixing of two identical colliding droplets are restricted by the intrinsic symmetry across the plane of collision, and that droplets with either disparity in the physical properties

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Nomenclature

C	fluid composition
D	droplet diameter
E_0	bulk free energy
k	gradient factor
L_0	initial distance between the droplets
M	mobility of the interface
p	pressure
t	time
t_0	time of initial coalescence
t_{osc}	characteristic oscillation time of the smaller droplet, $t_{osc} = \sqrt{\rho_l D_S^3/\sigma}$
t^*	normalized time, $t^* = (t - t_0)/t_{osc}$
$\boldsymbol{u}$	flow velocity
U_0	initial relative velocity between the droplets
$\boldsymbol{U}$	initial velocity of the droplet
β	prefactor of the bulk free energy
ξ	thickness of the liquid-gas interface
ρ	density
μ	dynamics viscosity
μ_C	chemical potential
σ	surface tension coefficient

Subscripts

L	larger droplet
S	smaller droplet
l	liquid phase
g	gas phase

Nondimensional parameters

We	*Weber* number, $We = \rho_l U_0^2 D_S/\sigma$
Oh	*Ohnesorge* number, $Oh = \mu_l/\sqrt{\rho_l D_S \sigma}$
Δ	size ratio, $\Delta = D_L/D_S$
ρ^*	density ratio, $\rho^* = \rho_l/\rho_g$
μ^*	viscosity ratio, $\mu^* = \mu_l/\mu_g$

or in the sizes may result in enhanced mixing by symmetry-breaking. In this regard, Blanchette [19] numerically observed increasingly significant mixing between two equal-sized droplets with surface tension difference as the result of the Marangoni effect. Focke et al. [20] investigated both experimentally and numerically on the collision dynamics of droplets with viscosity disparity and observed enhanced mixing. Sun et al. [21] numerically simulated the collision of two non-Newtonian droplets and found that the internal mixing is promoted for the droplets with significant rheological difference. Specifically, liquid interpenetration is facilitated for the droplets with different extent of shear-thinning effect, while permanent coalescence and internal mixing are simultaneously facilitated for the collision between a shear-thinning droplet and a shear-thickening droplet.

Compared with the collision between droplets with distinct physical properties, unequal-sized droplet collision has attracted more attention particularly due to its higher practical relevance, not to mention its intrinsic tendency of promoting permanent coalescence, which is required by the subsequent internal mixing [6]. Anilkumar et al. [22] experimentally found that, the inertialess coalescence of a droplet and a liquid pool may lead to a jet-like mixing with an accompanied strong vortex ring. Numerical simulations by Nobari and Tryggvason [23] and Liu et al. [24] show that the jet-like mixing is largely affected by the droplet viscosity and can form only at sufficiently small *Ohnesorge* numbers. Sun et al. [25] further justified that the formation of the jet-like mixing depends on whether the viscous damping on the capillary wave propagation is small enough to allow a liquid bulge to form before the smaller droplet totally merges into the large one. As a result, lowering the viscosity of the smaller droplet rather than that of the larger droplet is much more effective in facilitating the jet-like mixing. Xia et al. [26] analyzed the generation of vorticity inside the merged droplet and found that the emergence of the internal jet is attributed to the formation of a main vortex ring, as the jet-like structure shows a strong correlation with the main vortex ring.

The collision dynamics and internal mixing at larger impact inertia were investigated experimentally by Ashgriz and Poo [27], and numerically by Nikolopoulos et al. [28,29], Sun et al. [30], and Chen et al. [31]. It is noteworthy that the jet-like mixing was also numerically observed at high *Weber* numbers as long as the *Oh* number is sufficiently small [30,31] and was experimentally confirmed by Tang et al. [32] recently. Their experiments also show the interesting non-monotonic emergency of "jet" – "no jet" – "jet" as the impact inertia increases, suggesting that the two types of jet may be owing to different mechanisms. The experiment by Zhang et al. [33] on the hypergolic ignition by head-on collision of N,N,N′, N′-tetramethylethylenediamine and white fuming nitric acid droplets further showed a non-monotonic variation of the ignition delay times with increasing the *We* number. This phenomenon was attributed to the non-monotonic emergence of jet-like mixing, which facilitates the liquid-phase reactions. It is nevertheless noted that, compared to the surface-tension-induced jet-like mixing identified in low *We* number collisions/coalescences, the collision-induced jet-like mixing at high *We* number collisions still remains inadequately understood.

In the present investigation, we aim to numerically study the high-*We*-number collision of unequal-sized droplets, with particular interest in the formation of internal jet that facilitates mixing. Only head-on collision is taken into consideration, since the jet-like mixing for eccentric droplet collision was not observed either in the experiment of Ashgriz and Poo [27] or in the numerical simulation of Chen [31], indicating the emergence of internal jet does not favor the eccentricity between the droplets. In the following text, the numerical methodology, results and discussion, and concluding remarks are presented sequentially in Sections 2–4.

2. Numerical methodology

2.1. Problem specifications

Since the head-on droplet collision is intrinsically symmetric with respect to the axis connecting the centers of mass of the two droplets, an axisymmetric computational domain is employed in the present study. As shown in Fig. 1, two droplets of diameter D_S and D_L (the subscripts S and L denote small and large, respectively) are placed in the initially stationary gaseous environment, with their velocities given by $\boldsymbol{U}_S = -(D_L/D_S)^3 \boldsymbol{U}_L$ so as to zero the total momentum of the binary system. The outflow boundary condition is applied on the domain boundaries except the axis.

2.2. Macroscopic governing equations

In the present study, the phase-field multiphase model [34,35] is employed to capture the liquid-gas interface. The composition C,