Numerical simulation of the head-on collision of two equal-sized drops with van der Waals forces

Xueli Jiang and Ashley J. James*

University of Minnesota,
Department of Aerospace Engineering and Mechanics,
Minneapolis, Minnesota, 55455

Abstract

The head on collision of two equal-sized drops driven by a hyperbolic flow is investigated numerically. An axisymmetric volume of fluid (VOF) method is used to simulate the motion of a drop toward a symmetry plane where it interacts with, and possibly coalesces with, its mirror image. The volume fraction boundary condition on the symmetry plane is manipulated to numerically control coalescence. It is well known that the van der Waals forces become important and govern coalescence when the thickness of the fluid film between the two drops is sufficiently thin. Two new numerical methods have been developed to include the van der Waals forces into the Navier-Stokes equations. One method applies a body force to the drop which is computed as the negative gradient of the van der Waals potential. The other method calculates the van der Waals forces in terms of a disjoining pressure in the film which depends on the film thickness. This method is compared to theory of the rupture of a fluid film. The evolution of the film between the drops is studied both with and without the van der Waals forces included, and the results are compared. The influence of the van der Waals forces on the evolution and rupture of the film is examined. Comparisons of the results of the two methods at various values of the Hamaker constant show that the van der Waals forces calculated from the two methods have qualitatively similar effects on coalescence.
I. INTRODUCTION

Drop collision is a basic and important phenomenon encountered in a wide range of processes. Rain drop formation is one of the examples in nature. Numerous applications involving drop collisions can also be found in industry. In polymer blending, coalescence and break up of liquid particles are fundamental in governing the development of the blend’s morphology which determines the physical properties of a blend. In spray combustion, frequent collisions of drops in the dense spray region near the injector can significantly affect drop size and velocity, and thus the ultimate combustion performance. Abundant examples of drop collision also exist in various other fields, such as liquid-liquid extraction, ink-jet printing, drug delivery, and waste treatment.

Due to its significance, drop collision has been of interest to researchers for decades. However, most studies have been limited to experiments because of the complex physics and the wide range of length scales in this process. Literature on experimental investigations of collision problems is extensive. According to previous studies, binary collision outcomes can be generally divided into four regimes: bouncing, in which two drops collide and bounce apart; coalescence, in which two drops merge permanently forming a single drop; separation, in which drops coalesce temporarily and then split into two drops again; and fragmentation, in which small satellite drops are formed during separation of the temporarily coalesced drops.

Many efforts have been made to understand the characteristics of different collision behaviors, the boundaries separating them and the physics behind them. Ashgriz & Poo conducted extensive experiments on coalescence and separation collisions. The regimes of coalescence and two different types of separation characterized by the impact parameter, namely reflexive separation for small impact parameters and stretching separation for large impact parameters, were found in the space of Weber number and impact parameter. A systematic experimental study of collision dynamics of equal-sized water and hydrocarbon drops was performed by Jiang et al. Boundaries between different collision outcomes for five different hydrocarbons were delineated, which showed significant differences from those of water drops. Energy dissipation during the collision process as well as the effects of the material properties of the fluids on collision behaviors were analyzed. Qian & Law extended Jiang’s study and investigated the effects of the ambient gas, including gas pressure, viscos-
ity, molecular weight, and molecular structure, on the transition between different collision regimes. They also presented a coalescence/separation criterion for head-on collisions. A review of experimental studies of water and fuel drop collision dynamics can be found in Ref. 1. Some researchers\textsuperscript{5,6} investigated coalescence of drops in linear flows generated by a four roll mill. The recent experimental studies of this kind were reviewed by Leal.\textsuperscript{7}

Unlike experiments, numerical simulations have the potential advantage of being able to resolve the thin film between the drops. However, numerical investigations of binary drop collisions are rare. Poo & Ashgriz\textsuperscript{8} presented simulations of drop collision, but their study was limited to two dimensions and bouncing collisions were not studied. Mashayek \textit{et al.}\textsuperscript{9} employed a spine-flux method and focused their study on coalescing collisions of two drops colliding head-on under a fixed Weber number of 1. The effects of Reynolds number, internal circulation and drop size ratio on coalescence were examined. Unlike most of the studies that did not give much attention to bouncing or were unable to simulate bouncing, Nobari \textit{et al.}\textsuperscript{10} investigated both bouncing and non-bouncing outcomes of head-on collisions of two equal-sized drops using a front tracking method. The velocity and pressure field inside the bouncing drops were studied in detail. The effects of Reynolds number and Weber number were examined. However, in their study, coalescence did not happen naturally, but by artificially removing the thin film between the drops. The time when the film was ruptured was found to affect the behavior of the combined drop. A three-dimensional version of the same method was used to simulate off-center binary collisions by Nobari & Tryggvason.\textsuperscript{11} Three-dimensional computations of drop collision have also been published by Lafaurie \textit{et al.}\textsuperscript{12} who employed a volume of fluid (VOF) method, but they mainly focused on introduction of the method rather than the collision dynamics. Zinchenko \textit{et al.}\textsuperscript{13} presented a three-dimensional boundary integral method to simulate gravity-induced interaction of drops at low Reynolds numbers. The drops could become arbitrarily close to each other, but could not coalesce in their method. In addition to the traditional approaches based on the continuum concept, the method of molecular dynamics has also been used to study collision dynamics.\textsuperscript{14,15} In this method, the intermolecular forces which govern the gross motion of a fluid are modeled. Thus collision outcomes happen naturally. However, since drops are represented by discrete particles, the exact shape of an interface is hard to determine. Furthermore, because of its computational intensity, this method can only simulate very small drops and collisions over extremely short times.
When two equal-sized drops immersed in an immiscible fluid approach each other along the axis of their centers, a film forms between them and subsequently thins. When the thickness of the film falls into the range of several hundreds of Angstroms, 100-1000 Å, van der Waals forces become significant, leading to rupture of the film and consequently coalescence of the drops.

The literature in van-der-Waals-driven thin film rupture is rich, but most of the studies are focused on rupture of a free film,\textsuperscript{16,17} or a thin film on a solid substrate.\textsuperscript{18,19} Studies on thinning and rupture of a thin film between drops, which is usually dimpled, in coalescence collisions are limited. Lin & Slattery\textsuperscript{20} studied the drainage of a liquid film between a small drop or bubble and a fluid-fluid interface. The van der Waals forces were neglected since the film was considered to be sufficiently thick. To simplify the problem, the Reynolds number was assumed to be small and the lubrication approximation was used. Chen & Slattery\textsuperscript{21} extended Lin & Slattery’s theory by adding the van der Waals forces which were represented in terms of a scalar potential in the equation of motion. Based on the same model, Hahn et al.\textsuperscript{22} examined the thinning and rupture of a liquid film between a drop and a fluid-fluid interface under the influence of van der Waals forces. The existence of the van der Waals forces was found to decrease coalescence time. Chen\textsuperscript{23} further extended this model by including the electric double layer effect and used the model to simulate the coalescence between two equal-sized drops during head-on collision with emphasis on drainage and rupture of the film between the two drops. The evolution of the film shape and the effect of different strengths of van der Waals forces on the rupture time were presented. Yianitsios and Davis\textsuperscript{24} examined the effects of van der Waals forces on the rupture process of the film between two different-sized drops as they approach each other due to gravity at small capillary number. The van der Waals forces were applied in the form of a negative disjoining pressure on the interface as a boundary condition. Lubrication theory was applied in the film. They found that large van der Waals forces lead to ‘nose rupture’ on the symmetry axis and small van der Waals forces lead to off-center ‘rim rupture’.

In this study, we present the numerical simulation of the collision of two equal-sized drops driven by a hyperbolic flow. The effects of van der Waals forces on the coalescence of the drops are examined. The van der Waals forces are calculated by two different methods. In one method, a body force acting on the drops and calculated from an interaction potential is introduced into the momentum equation.\textsuperscript{25} In the other method a disjoining pressure in
the film is used to represent the van der Waals forces as in Refs. 16,17,23. The concept of
disjoining pressure which accounts for the pressure difference between a thin film and the
bulk phase from which the film is made was first introduced by Deryagin.26

The primary difference between our research and previous work is that the Reynolds
number and capillary number need not be small as in most of the other theoretical and
computational studies. The full Navier-Stokes equations, with modifications to represent
van der Waals forces, that govern the motion of the fluid both inside the drop and in the
surrounding flow are solved. In addition, we examine the whole coalescence process from
the approach of the two drops to the rupture of the film, and to the formation of the single
drop. We start with two drops separated by some distance and the film between the drops
develops naturally. Our goal is to develop a numerical model that can accurately simulate
the collision of two drops and give us a better understanding of the dynamics.

The paper is organized as follows. Sec. II presents the problem studied, the governing
equations, and the numerical methods. The two methods used to incorporate van der Waals
forces are introduced in Sec. III. The results are reported in Sec. IV. Sec. V is devoted to
conclusions.

II. FORMULATION

Two equal-sized spherical liquid drops are immersed in an axisymmetric extensional gas
flow, as shown in Fig. 1. The drops are centered on the symmetry axis of the flow. Driven
by the suspending fluid, the drops will collide head-on and then may bounce apart or come
into contact.

An axisymmetric volume of fluid (VOF) method is used to simulate the collision process
of the two drops. The VOF method was first developed by Nichols, Hirt & Hotchkiss27
and Hirt & Nichols.28 In this method, a volume fraction, \( F \), is defined in each cell as the
fraction of the volume of the cell containing liquid. Thus \( F \) is one inside the drops and
zero inside the gas. Other values of \( F \) represent an interface. The geometry of the interface
is approximated by reconstructing the interface based on the volume fraction data. The
motion of the interface is captured through the evolution of the volume fraction.

The fluid in the drops and in the ambient gas is considered as a whole and one set of
equations that govern the motion in the whole domain is used. The effort of applying bound-
ary conditions on the free surface is then saved, but the surface tension must be accounted for correctly. For this purpose, the continuum surface force (CSF) method introduced by Brackbill et al.\textsuperscript{20} is employed to calculate the surface tension. In this method, the volume fraction is smeared over a small region near the interface. The surface tension is treated as a volume force that varies continuously across the interface with nonzero values only in the smeared region near the interface. As the grid is refined and the thickness of this region goes to zero, the surface tension retrieves its exact value. For constant surface tension coefficient $\sigma$, the volume force used to simulate surface tension can be expressed as $\sigma \kappa \nabla F$, where $\kappa$ is the interface curvature.

For incompressible, transient, interfacial flows, the axisymmetric dimensionless governing equations are the continuity equation,

$$\frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial v}{\partial z} = 0,$$

the Navier-Stokes equations,

$$\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + v \frac{\partial u}{\partial z} \right) = -\frac{\partial p}{\partial r} + \frac{1}{Re} \left[ 2 \frac{\partial }{\partial r} \left( \mu \frac{\partial u}{\partial r} \right) ight. $$

$$\left. + \frac{\partial }{\partial z} \left( \mu \frac{\partial v}{\partial r} + \mu \frac{\partial u}{\partial z} \right) + 2 \mu \frac{\partial }{\partial r} \left( \frac{u}{r} \right) \right]$$

$$+ \frac{\kappa}{We} \frac{\partial F}{\partial r} + f_{vr}$$

$$\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial r} + v \frac{\partial v}{\partial z} \right) = -\frac{\partial p}{\partial z} + \frac{1}{Re} \left[ \frac{\partial }{\partial z} \left( \mu \frac{\partial v}{\partial z} \right) \right. $$

$$\left. + \frac{\partial }{\partial r} \left( \mu \frac{\partial v}{\partial r} + \mu \frac{\partial u}{\partial z} \right) + \frac{\mu}{r} \left( \frac{\partial v}{\partial r} + \frac{\partial u}{\partial z} \right) \right]$$

$$+ \frac{\kappa}{We} \frac{\partial F}{\partial z} + f_{vz},$$

and the volume fraction convection equation,

$$\frac{\partial F}{\partial t} + u \frac{\partial F}{\partial r} + v \frac{\partial F}{\partial z} = 0,$$

where $u$ is the velocity in the radial direction, $v$ is the velocity in the vertical direction, $\rho$ is the density, $\mu$ is the viscosity, $p$ is the pressure, $Re$ is the Reynolds number, $We$ is the Weber number, and $f_{vr}$ and $f_{vz}$ are the radial and vertical components of the van der Waals forces $\vec{f}_v$. Gravity is neglected. The calculation of van der Waals forces will be introduced in the next section.
The length scale used in non-dimensionalization is the radius of the drop, \( R \). The velocity scale is the strain rate of the hyperbolic flow, \( G \), times \( R \). Inertial time and pressure scales are used. The density and viscosity are scaled on the density of the drop \( \rho_d \) and the viscosity of the drop \( \mu_d \), respectively.

The non-dimensional parameters are the Reynolds number, \( Re = \rho_d G R^2 / \mu_d \), the Weber number, \( W_e = \rho_d G^2 R^3 / \sigma \), the Hamaker number if van der Waals forces are considered, \( A = \bar{A} / \rho_d R^6 G^2 \), where \( \bar{A} \) is the Hamaker constant, the density ratio, \( \alpha = \rho_o / \rho_d \), and the viscosity ratio, \( \beta = \mu_o / \mu_d \), where \( \rho_o \) and \( \mu_o \) are the density and viscosity of the surrounding gas, respectively.

The flow field is solved by a projection method\textsuperscript{30,31} on a staggered grid. The resulting pressure-Poisson equation is solved using an incomplete Cholesky conjugate gradient method.\textsuperscript{32} The volume fraction is convected by calculating the volume flux across each cell face. The interface is reconstructed from the volume fraction field at each time step using a piece-wise linear approximation. Coalescence is considered to occur when any of the linear interface segments intersect the symmetry plane. The code, aside from the van der Waals forces, was thoroughly tested and used to study the breakup of a vibrating drop by James \textit{et al.}\textsuperscript{31}

As shown in Fig. 1, the \( z \) axis is a symmetry axis and \( z = 0 \) is a symmetry plane. To take advantage of symmetry, only the upper right quadrant is used as the computational domain, shown as the shaded region in Fig. 1. Initially the two drops are placed on the axis of symmetry with their centers separated by four radii. The velocity of the flow field is initialized as \( u = r \) and \( v = -2z \). This velocity is then maintained on the top and right boundaries. Symmetry conditions are imposed on the other boundaries. Boundary conditions for the pressure change between the current and next time step are derived from the velocity boundary conditions. In this case, the derivative of the pressure change normal to each boundary is zero.

The volume fraction is zero at the top and the right boundaries, and symmetric about the symmetry axis. Special attention is paid to the volume fraction boundary condition on the symmetry plane. Since only one of the drops' profiles is used, the drop in the computational domain interacts with its mirror image through the volume fraction boundary condition on the symmetry plane. Therefore the volume fraction boundary condition plays a significant role in modeling the collision behavior. Based on the physics of the collision, two kinds of
the volume fraction boundary conditions are used: $F = 0$ and $\partial F/\partial z = 0$, which will lead to different collision outcomes. Details of the results will be discussed in Sec. IVB.

The volume fraction boundary conditions are applied using the ghost cells just outside the physical boundaries, as shown in Fig. 2. The volume fraction in each ghost cell will be set to be zero if the zero boundary condition is used, and will be equal to the volume fraction in the adjacent real cell if the symmetry boundary condition is used. If the volume fraction in the ghost cells is zero, the drop in the computational domain can not ‘see’ the mirror drop. It can only ‘see’ the boundary as a non-wetting slip wall. However, symmetry conditions for the velocity and pressure mimic collision. Consequently the drop can not merge with the mirror drop and it will bounce. In general, in the VOF method, two interfaces will merge automatically whenever they are closer than the cell size. If the symmetry boundary condition is used, this leads to coalescence of the drops. Unfortunately the information of the mirror drop will interfere with the reconstruction of the interface of the simulated drop as well as the computation of curvature and in turn the surface tension. In our simulations, the usage of symmetry and zero conditions enables us to simulate not only coalescence but also bouncing. However, resolution of the two separate, but nearby, interfaces in the coalescing case is somewhat problematic. Future work will address this issue.

III. CALCULATION OF VAN DER WAALS FORCES

We have developed two different methods to calculate the van der Waals forces. One method represents the van der Waals forces as the interaction force between the drops. The other one accounts for the van der Waals forces as a disjoining pressure in the film between the drops.

In the first method, the interaction potential between the two drops due to the van der Waals forces is computed first. Then a body force acting on the drop is calculated as the negative gradient of the van der Waals potential. The body force, which is attractive since the two drops are of the same material, is then introduced into the momentum equation. Since the flow in the whole domain is computed simultaneously, the body force exerts its influence on the thinning and rupture of the film between the drops via the interface.

Numerically the van der Waals forces $f_v$ are calculated as follows. The potential energy between the two drops is calculated via a microscopic Hamaker procedure. Here the
interactions with gas molecules are neglected.

The potential energy of a molecule located in the cylindrical cell \((m,n)\) in the simulated drop \(i\) due to a molecule in the cell \((s,t)\) in the mirror drop \(j\) is

\[-\lambda_{ij}/L^6,\]  

(5)

where \(\lambda_{ij}\) is the dimensionless London constant, which is linked to the London constant \(\tilde{\lambda}_{ij}\) as \(\lambda_{ij} = \tilde{\lambda}_{ij}/\rho_dR^{11}G^2\), and \(L\) is the distance between the two molecules, as shown in Fig. 3. For small grid spacings, it can be approximated that the two molecules are at the centers of the two cells. \(L\) then becomes

\[L = \sqrt{H^2 + (r_m^2 + r_s^2 - 2r_m r_s \cos \theta)},\]  

(6)

where \(r_m\) and \(r_s\) are the radial coordinates of the centers of the cells \((m,n)\) and \((s,t)\), respectively, \(H\) is the perpendicular distance between the two molecules, and \(\theta\) is shown in Fig. 3.

The potential energy of a molecule in the cell \((m,n)\) due to all the molecules in the cell \((s,t)\) is obtained by multiplying Eq. 5 by the volume fraction in \((s,t)\), \(F_{st}\), and the number of molecules per dimensionless unit volume in the drop \(j\), \(N_j\), and integrating over the cell volume,

\[d\phi_{mn} = \int_{\text{cell } (s,t)} -\frac{\lambda_{ij}}{L^6} N_j F_{st} r dr d\theta dz,\]  

(7)

where \(N_j\) is related to its dimensional form \(\tilde{N}_j\) as \(N_j = R^3 \tilde{N}_j\). Eq. 7 is approximated as

\[d\phi_{mn} \approx -\lambda_{ij} N_j r_s \Delta r \Delta z F_{st} \int_0^{2\pi} \frac{1}{L^6} d\theta,\]  

(8)

for small grid spacings in the \(r\) and \(z\) directions, \(\Delta r\) and \(\Delta z\), respectively. The integration \(\int_0^{2\pi} 1/L^6 d\theta\) can be evaluated as

\[\int_0^{2\pi} \frac{d\theta}{L^6} = 2\pi \left\{ \frac{(H^2 + r_s^2 + r_m^2)^2 + 2r_s^2 r_m^2}{[(H^2 + r_s^2 + r_m^2)^2 - (2r_s r_m)^2]^{5/2}} \right\}.\]

Thus,

\[d\phi_{mn} = -2\pi \lambda_{ij} N_j r_s \Delta r \Delta z F_{st} \times \left\{ \frac{(H^2 + r_s^2 + r_m^2)^2 + 2r_s^2 r_m^2}{[(H^2 + r_s^2 + r_m^2)^2 - (2r_s r_m)^2]^{5/2}} \right\}.\]
The potential energy per unit volume in cell \((m, n)\) due to the entire drop \(j\) is computed by summing over all the cells in \(j\),

\[
\phi_{mn} = -2\pi \lambda_{ij} N_i N_j \Delta r \Delta z \times \sum_{s,t} \left\{ r_s F_{st} \left[ (H^2 + r_s^2 + r_m^2)^2 + 2r_s r_m^2 \right] \right\} \times \frac{\left( (H^2 + r_s^2 + r_m^2)^2 + 2r_s r_m^2 \right)}{\left( (H^2 + r_s^2 + r_m^2)^2 + (2r_s r_m)^2 \right)^{3/2}},
\]

where \(N_i\) is the number of molecules per dimensionless unit volume in drop \(i\), which is related to its dimensional form \(N_i = R^3 N_i\), and \(\lambda\) is the dimensionless Hamaker constant, which is related to the Hamaker constant \(A\) as \(\lambda = A / \rho d R^6 G^2\), where \(\lambda = \pi^2 N_i N_j \lambda_{ij}\).

The force per unit volume at \((m, n)\) is

\[
\vec{f}_v = -F_{mn} \nabla \phi_{mn},
\]

where \(\phi\) is computed from Eq. 9 and central differencing is used to evaluate Eq. 10. This force is weighted by the volume fraction in that cell, \(F_{mn}\), to ensure that the force occurs only inside the drop.

In the other method, the effect of van der Waals forces on the film is incorporated as a disjoining pressure in the film. According to Deryagin,\(^{26}\) the disjoining pressure can be introduced into the equation of motion. For a plane-parallel film with a thickness of \(h\), the disjoining pressure is given by\(^{24, 25, 34}\)

\[
\Pi(h) = -\frac{A}{6\pi h^3}.
\]

The gap between the two drops is not uniform, especially when the distance between the drops is large, but we assume that the van der Waals forces are negligible when the drops are far away. When the drops are close enough for the van der Waals forces to be important, we assume that the thickness of the film changes gradually so that the slope of the interface is small. It is then appropriate to use Eq. 11 to approximate the disjoining pressure in the film. The validity of this assumption will be examined in Sec. IV C.

The van der Waals force reads

\[
\vec{f}_v = -\nabla \left( \frac{A}{6\pi h^3} \right).
\]
Since the disjoining pressure depends on the thickness of the film only, inside the film

\[ \frac{\partial}{\partial z} \left( \frac{A}{6\pi h^3} \right) = 0. \]  \hspace{1cm} (13)

The van der Waals forces are then

\[ \vec{f}_v = -\frac{\partial}{\partial r} \left( \frac{A}{6\pi h^3} \right) \vec{r}, \]  \hspace{1cm} (14)

which is evaluated using second-order central differencing. In the computation, the film thickness \( h \) is defined only inside the film between the drops. It is calculated as the average height of the liquid in a cell column. A cutoff of \( h = 10^{-4} \) based on experience is introduced to keep the code from blowing up as \( h \to 0 \).

IV. RESULTS AND DISCUSSION

In this section, the calculation of the van der Waals forces is validated first. Then the results of the drop collision problem are presented in the absence of the van der Waals forces. The significance of the volume fraction boundary condition on the symmetry plane is discussed. Finally the results with the van der Waals forces are reported.

A. Code validation

To verify our algorithms for calculating van der Waals forces, we simulate the van-der-Waals-driven axisymmetric point rupture of a free film and compare with previous results\textsuperscript{17}. The case which has been examined by Vaynblat et al.\textsuperscript{17} using a long-wavelength model is considered. Vaynblat et al. have confirmed numerically that near the rupture time \( t_c \) and the rupture point \( r_c \), the solutions to the long-wavelength lubrication equations\textsuperscript{17} describing the rupture have the similarity forms

\[ h(r, t) = \tau^\alpha H(\eta) \]  \hspace{1cm} (15)

\[ u(r, t) = \tau^\gamma U(\eta), \]  \hspace{1cm} (16)

where \( \tau = t - t_c, \eta = (r - r_c)/\tau^\beta \), and the constants \( \alpha, \beta, \gamma \) are scaling exponents. Dimensional analysis based on the continuity equation gives

\[ \gamma - \beta = -1. \]  \hspace{1cm} (17)
The dynamic balance they made between van der Waals forces, viscosity and inertia while surface tension neglected results in the following scaling exponents

\[ \alpha = 1/3, \quad \beta = 1/2, \quad \gamma = -1/2. \] (18)

They solved the lubrication equations numerically on a highly adaptive mesh and verified the above values for the scaling exponents.

We adopt the same problem, but solve the full Navier-Stokes equations in the axisymmetric coordinate system. It is difficult to implement the potential method to compute the van der Waals forces because the film is infinite and the coordinate system is axisymmetric. Therefore, only the disjoining pressure method is used in the simulation. As we shall see in part C of this section, the potential method gives similar results to the disjoining pressure method for the drop coalescence problem.

The characteristic scales are: length \( h_0 \), velocity \( \mu/\rho h_0 \), time \( \rho h_0^2/\mu \), and pressure \( \mu^2/\rho h_0^2 \), where \( h_0 \) is the mean thickness of the film, \( \rho \) is the density of the film, and \( \mu \) is the viscosity of the film. To compare with the results in Ref. 17, the dimensionless parameter values in our scaling are

\[ Re = 1, \quad We = \pi^2/3, \quad \text{and} \quad A = 6\pi^2, \] (19)

where \( \epsilon \) is the ratio between the mean thickness of the film and the lateral length of the film. The effect of varying the parameter \( \epsilon \) will be considered. Since the film in Ref. 17 is in a vacuum environment, a small value is chosen for the density and viscosity ratios: \( \alpha = \beta = 0.01 \). Additional simulations showed that this value is sufficiently small to have no effect on the results.

To take advantage of symmetry, only a quarter of the film profile is used as the computation domain which is taken to be \([0, 1/\epsilon] \times [0, 1]\). The initial film profile is the same as in Ref. 17. In our non-dimensional variables, the half film thickness is \( 0.5h(r, 0) = 0.5 - 0.1 \cos(\epsilon \pi r) \). The calculation in Ref. 17 is one dimensional, so only the velocity in the \( r \) direction, \( u \), is defined and initially is \( u = 0.1\epsilon \sin(\epsilon \pi r) \). In our simulation, this initial condition for \( u \) is used in the film. The initial \( v \) velocity in the film and the velocity in the gas are derived based on the continuity equation. Since the similarity solution is independent of the initial conditions, we should be able to obtain the same similarity solution even though we use a slightly different initial condition. Other forms of initial conditions have also been
tested, but results show that while different initial conditions affect the rupture time, they have little effects on the similarity solution.

As a representative example, Fig. 4 shows the time evolution of the film for $\epsilon = 1/4$. The scaling exponents can be estimated from log-log plots of appropriate variables as in Ref. 17. For example, the slope of $-\partial h / \partial t(0,t)$ versus the minimum film thickness $h(0,t)$ on a log-log scale is $(\alpha - 1)/\alpha$, whose theoretical value is $-2$. Similarly $\partial^2 h / \partial r^2(0,t)$ gives $(\alpha - 2\beta)/\alpha = -2$, and $\partial u / \partial r(0,t)$ gives $(\gamma - \beta)/\alpha = -3$. Fig. 5 shows the log-log plots of the above variables as functions of $h(0,t)$ for $\epsilon = 1/4$. All variables approach linear behavior in the late stages of the thinning of the film, which proves the existence of the similarity solution.

A systematic study has been conducted for different values of $\epsilon$ and different grid resolutions. In Ref. 17, $\epsilon \ll 1$ is the basic assumption for the lubrication model. However, since the full Navier-Stokes equations are solved in our simulation, the computational cost prevents us from using very small $\epsilon$ as well as very fine grids which are important for resolving the thin film near rupture. Despite of these limitations, by varying $\epsilon$ and the resolution we can show that our results approach the ones in Ref. 17 as $\epsilon$ decreases and as the resolution is refined.

The computed slopes of $-\partial h / \partial t$ and $\partial u / \partial r$ and the exponents estimated from these slopes are summarized in Table I and Table II. The slopes have a reasonable agreement with the theoretical values. Therefore, the constant $\alpha$ and the relationship in Eq. 17 are reproduced. However, the slope of $\partial^2 h / \partial r^2$ differs from its theoretical value, and it is consistent with the previous work of Ida and Miksis. The main reason for this discrepancy is resolution. As discussed by Vaynblat et al., when surface tension is small compared with viscosity, as in the current case, a transition region, in which the inertial effects are sub-dominant, exists before van der Waals forces, viscosity and inertia all balance. Ida and Miksis have made the balance between van der Waals forces and viscosity while neglecting inertia, which led to $\alpha = 1/3$ while $\beta$ and $\gamma$ were undermined. The results of their simulation of the line rupture of a free film under the same parameters supported this scaling. However, Vaynblat et al. pointed out that the value of $\beta$ estimated from the results of Ida and Miksis did not fall into the range required by this scaling. Furthermore, Vaynblat et al. were able to resolve the film up to $10^{-10}$ compared to $10^{-3}$ in Ida and Miksis’s study, which enabled Vaynblat et al. to confirm that the balance at the final rupture stage is between van der Waals forces,
viscosity and inertia. Vaynblat et al. also observed that $\vartheta^2 h/\vartheta r^2$ took a longer time to approach linear behavior than other variables, which showed the existence of the transition region. Therefore, Vaynblat et al. concluded that the simulation of Ida and Miksis was still in the transient region. Due to computational intensity, the smallest film thickness we can resolve is about $10^{-2}$. Our calculated value of $\beta$ is $0.37 \sim 0.38$ which is close to the value of 0.39 in the results of Ida and Miksis. Considering the observation of Vaynblat et al., we conclude that our calculation has not reached the eventual rupture region, hence the values of $\beta$ and $\gamma$ observed disagree with the theoretical values in Eq. 18.

B. Symmetry condition

In the rest of the simulations, $\alpha$ and $\beta$ are both specified as 0.001. $Re = 1$, $We = 1$ are used so that the effects of inertia, viscosity and surface tension are of equal importance.

As discussed in Sec. II, unlike the other variables, the volume fraction has selective boundary conditions on the symmetry plane. Different boundary conditions are used to model different collision behaviors. Fig. 6 gives a general picture of the coalescence collision. In this case, the symmetry boundary condition is used. As a result, the drop and its image merge automatically. Note the computational domain, comprised of $100 \times 200$ grid cells, encompasses the upper right quadrant only, but its mirror images are shown for clarity. The straight-line approximation in each interfacial grid cell is plotted, which is necessary to represent the interface correctly near the symmetry plane.

It is well known$^{23,24}$ that as two drops approach each other the pressure between them builds up, leading to the formation of a dimple, as shown at $t = 0.37$ in Fig. 6. At $t = 0.40$, coalescence occurs at the rim of the dimple, resulting in high curvature at the contact point and subsequently a large surface tension force there. The contact area is then increased by surface tension, leaving a bubble trapped in the center. After the post-collision drop has reached its maximum deformation at $t = 0.80$, it and the entrapped bubble relax to a rounder shape. In this figure the gross motion of the two drops is captured, but some of the details are not physical due to the limitation of the axisymmetry. For instance, experimentally it is seen that azimuthal instabilities lead to coalescence at a point, not along the entire ring that surrounds the dimple. However, azimuthal variations are not allowed in this simulation. This limitation also allows the formation of toroidal bubbles in the simulation, which is certainly
non-physical.

Details of the evolution of the film between the drops are shown in Fig. 7(a). This figure shows the half thickness of the film between the drops, $h/2$, as a function of time and radial position. It can be seen that the interface translates downward with little deformation until $t = 0.29$ when the interface near the symmetry axis flattens. After that a dimple forms and grows rapidly, the minimum thickness of the film decreases, and the film ruptures at the rim of the dimple at $t = 0.40$.

Fig. 7(b) shows the pressure at the symmetry plane as a function of time and radial position. It illustrates the pressure evolution in the film between the drops. From $t = 0.27$ to $t = 0.29$, there is a dramatic increase in pressure at the symmetry axis. The pressure peak then moves radially outward with the dimple. The thinning rate at the symmetry axis slows down under such a sudden increase of pressure, as shown in Fig. 8. The film at the symmetry axis thins quickly until a transition point at about $t = 0.29$ and then thins slowly. The curves of half film thickness at the symmetry axis $h_c/2$ and half minimum thickness $h_{\text{min}}/2$ deviate at around the same time, indicating the formation of the dimple.

Fig. 9 shows the rebound of the two drops. The zero volume fraction boundary condition on the symmetry plane is used. Therefore the drop sees the boundary as a slip wall, but it cannot merge with its image. Impact of the drops creates a large pressure between them, so the drops rebound even though the applied velocity continues to force them toward each other. Fig. 10(a) provides detailed shapes of the film between the drops. Unlike the coalescence case, the dimpled film does not rupture, but flattens as the drops deforms. As the drops rebound, the film resumes its dimpled shape until the drops are almost round. Fig. 10(b) shows the pressure at the symmetry plane as a function of time and radial position, which is quite similar to Fig. 7(b).

As shown by the above results, by manipulating the volume fraction boundary condition on the symmetry plane, we can simulate both coalescence and bouncing. However, the current model can not predict whether these two drops should merge or bounce. This will be the subject of future work.
C. Effect of the van der Waals forces

When the film between the drops is sufficiently thin, the van der Waals forces become significant and destabilize the film. In this section we focus on the effects van der Waals forces have on the rupture of the film. For this reason, the symmetry volume fraction boundary condition is used on the symmetry plane and the van der Waals forces are turned off once coalescence happens. The dimensionless Hamaker number, $A$, is varied to adjust the strength of van der Waals forces. Three different values, which correspond to increasing strength of van der Waals forces, are used: $A = 0.1, A = 1$, and $A = 10$.

1. Van der Waals forces calculated from potential

Fig. 11 shows the evolution of the film between the drops for three values of $A$. Two modes of rupture are observed for different values of $A$: ‘rim rupture’\textsuperscript{24} where the film ruptures at the rim of the dimple, as in Fig. 11(a) and (b); and ‘nose rupture’\textsuperscript{24} where the film ruptures at the symmetry axis, as in Fig. 11(c). These two modes of rupture were also observed and discussed by Yiantsios & Davis\textsuperscript{24} and Rother et al.\textsuperscript{36} At relatively small $A$, for example $A = 0.1$, a dimple is formed and grows. However, the size of the dimple is smaller than the dimple in Fig. 7(a) in which $A = 0$. The size of the dimple continues to decrease as $A$ increases. At $A = 1$ only a very small dimple is formed. As $A$ is increased to 10, no dimple is formed at all. The rupture mode changes from rim rupture to nose rupture. This suggests that under strong van der Waals forces, the drops approach each other at such a fast rate that there is no time for a dimple to form.

Another fact apparent in Fig. 11 is that the rupture time decreases as the strength of the van der Waals forces grows. This point is also shown in Fig. 12 where the half minimum thickness of the film is shown as a function of time for different values of $A$. For small time, all the curves collapse with the curve $A = 0$, which implies that in this period of time van der Waals forces are weak. Thus the assumption that the van der Waals forces are negligible at large separation of the drops, which is used when introducing the disjoining method, is valid. As $A$ increases, the film thins faster, therefore the corresponding curve deviates from the $A = 0$ curve sooner. In addition, it can be seen that at small $A$, the curve of with van der Waals forces deviates at around the time when the dimple is formed. This implies that
the van der Waals forces become important at that time. Fig. 11 shows that the slope of the film is small after the dimple forms. This fact validates the second assumption in the disjoining method.

It is also interesting to note the change of the thinning rate of the film under different values of $A$. As mentioned in Sec. IV B, a transition point which is associated with the formation of the dimple exists, separating the faster thinning in early time and the slower thinning in later time, as shown on the curve $A = 0$. One expects that under stronger van der Waals forces the film thins faster. At $A = 0.1$, after the transition point, the film thins at a faster rate than the case of $A = 0$. At $A = 1$, the formation of the small dimple seems to have less effect on the thinning rate. The film thins more rapidly with a small change of thinning rate observed. When the van der Waals forces are strong, as $A = 10$, the curve deviates from the $A = 0$ curve early, indicating faster approach of the drops. No dimple forms to slow down the thinning of the film, so the transition point does not exist in this case. Close to the rupture time, the slope of the curve is large, which reveals the rapid drainage near the rupture time due to van der Waals forces.

2. *Van der Waals forces calculated from disjoining pressure*

Fig. 13 shows the evolution of the film between the drops for different values of $A$. Like in Fig. 11, rim rupture is observed for $A = 0.1$ and $A = 1$, and nose rupture for $A = 10$. Fig. 14 compares the curves of half minimum film thickness as a function of time obtained by the two methods and that without van der Waals forces. It can be seen that the results from the two methods are in reasonable agreement. Since the disjoining pressure method has been validated in Sec. IV A, the agreement of the two methods implies that the potential method is also valid.

Fig. 14 also shows that the film between the two drops thins faster in the case in which the van der Waals forces are calculated from the disjoining pressure. The form of the disjoining pressure is derived from the interaction potential between two semi-infinite liquid regions separated by a film of uniform thickness. The disjoining pressure is the force one of the regions exerts on a unit area of the other region. In applying this to the interaction of two drops, the assumption that the regions are semi-infinite is valid as long as the drop extent is relatively large, since the potential decreases as $L^{-6}$. The assumption that the interface is
flat leads to over-prediction of the van der Waals forces, and hence of the thinning rate. The disjoining pressure includes the effect a flat liquid region, but away from the current grid cell the film thickness is larger if the interface is convex, as it is near the contact point. Thus, the disjoining pressure accounts for the attraction of more nearby liquid than is actually present and over-predicts the attractive force.

V. CONCLUSIONS

In this paper the head-on collision of two equal-sized drops in a hyperbolic flow is studied numerically. Both coalescence and bouncing collisions are modeled and the effects of the van der Waals forces on coalescence are investigated. The evolution of the film between the drops is examined.

In our simulations, the two drops interact with each other on the symmetry plane through the volume fraction boundary condition which consequently affects the collision behavior dramatically. In the standard VOF method, coalescence happens automatically whenever two interfaces come within one grid cell of one other. Our simulations have shown that manipulation of the volume fraction boundary condition can be used to numerically control coalescence. A symmetry condition leads to coalescence while a zero condition leads to bouncing. In future work we will develop a physical model to properly control the boundary condition.

Two methods have been developed to calculate the van der Waals forces. One method incorporates the van der Waals forces in terms of the interaction potential between the two drops. The other one calculates the van der Waals forces from the disjoining pressure in the film between the drops. The two methods result in qualitatively similar behavior, but there are small quantitative differences in the results. For the simulations presented here the difference in the coalescence time ranges from 2.4% when $A = 10$ to 4% when $A = 0.1$. The value of $A$ for transition from rim to nose rupture lies in the same range in the two methods. The disjoining pressure method is much less computationally intensive, but relies on the assumption that the interface slope is small. These results show that disjoining pressure method captures the main features of the evolution, but may not provide adequate accuracy under all conditions.

The van der Waals forces take effect over a length scale that is much smaller than the
drop radius and result in rapid changes. Therefore, in the near contact area where the length scale is small and changes are fast, a fine grid is a necessity. Whereas away from this region, changes are not that pronounced, so a coarser grid is acceptable. In future work an adaptive mesh will be implemented in the current model so that the thin film between the two drops can be better resolved.

Additionally, in the future more extensive parameter studies will be performed and three-dimensional simulations will be performed.

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* Author to whom correspondence should be addressed


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TABLE I: Computed slopes and estimated exponents as a function of $\epsilon$. $\Delta r = \Delta z = 0.025$.

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<th>$\epsilon$</th>
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<th>$\gamma - \beta$</th>
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TABLE II: Computed slopes and estimated exponents as a function of grid resolution. $\epsilon = 1/3$.

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<td>-1</td>
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FIG 1. The physical problem and the computational domain (in grey). Two drops are propelled by a hyperbolic flow. The computational domain is comprised of $100 \times 200$ grid cells.

FIG 2. Illustration of the volume fraction boundary condition on the symmetry plane. (a) zero condition, (b) symmetry condition.

FIG 3. A molecule in cell $(m, n)$ in the simulated drop $i$ interacts with a molecule in cell $(s, t)$ in the mirror drop $j$.

FIG 4. Time evolution of an unstable thin film. A series of the film half-thickness is shown for $t = 0$ to $t = 26$ in increment of 2 units, and a final profile at $t = 27.70$ at the time of rupture. $\epsilon = 1/4, Re = 1, We = \pi^2/3, A = 3\pi/8$. The grid has $160 \times 40$ cells.

FIG 5. Log-log plots of $-\partial h/\partial t(0, t)$, $\partial^2 h/\partial r^2(0, t)$, and $\partial u/\partial r(0, t)$ for the case shown in Fig. 4. $\epsilon = 1/4, Re = 1, We = \pi^2/3, A = 3\pi/8$. The grid has $160 \times 40$ cells. Symbols are numerical data and solid lines are linear fits.

FIG 6. Coalescence of two drops. Van der Waals forces are absent. $\partial F/\partial z = 0$ boundary condition on the symmetry plane. $Re = 1, We = 1, \alpha = 0.001, \beta = 0.001$.

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FIG 8. Half film thickness at the symmetry line $h_c/2$ and half minimum thickness $h_{\text{min}}/2$ as a function of time. Van der Waals forces are absent. $\partial F/\partial z = 0$ boundary condition on the symmetry plane. $Re = 1, We = 1, \alpha = 0.001, \beta = 0.001$.

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FIG 12. Half minimum thickness of the film as a function of time under different values of $A$. $Re = 1, We = 1, \alpha = 0.001, \beta = 0.001$. (a) $A = 0.1$, (b) $A = 1$, (c) $A = 10$.

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(c) $A = 10$.

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