Numerical Investigation of Droplet Aerobreakup and Impingement Experiments at Mach 5

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Droplet simulations with and without phase change have been performed to further our understanding of the relevant physics involved in aerobreakup and impingement of water droplets at hypersonic flow speeds and large Weber numbers. The numerical simulations are conducted closely following light-gas gun experiments performed at the Southwest Research Institute. A robust higher-order WENO-based multiphase numerical method is used with the assumption of thermo-chemical equilibrium (infinitely fast relaxation) to enable simulations of the post-impingement phase. Adaptive mesh refinement allows for computationally efficient tracking of important flow features such as liquid/vapor/gas interfaces, shocks and wakes. The target geometry is modeled using an immersed boundary method. This paper aims to investigate the dominant physical mechanisms by simulating the problem considering different modeling fidelity such as with and without viscous effects and/or with and without phase change. This approach allows to explore how the droplet breakup is affected by these associated physical mechanisms. It was found that the vapor layer plays an important role in the droplet aerobreakup on the front face of the droplet as well as for the wake dynamics. The final droplet impingement phase could be robustly simulated with the current approach and, while not perfectly matching the experiment, the complexity of the relevant flow physics could still be investigated by comparing the simulation results with the experimental data.

I. Introduction

High-speed vehicles operating at lower altitudes or within higher altitude clouds may face adverse weather conditions, including rain or snow. These conditions pose a significant threat to the structural integrity of the vehicle. Predicting the aerodynamics accurately under such conditions is highly challenging due to the intricate interplay of various physical phenomena, including the interaction of multiple phases and fluid-structure dynamics. The ongoing research project focuses on investigating the interaction between droplets and the airflow surrounding vehicles moving at hypersonic speeds. As the droplet moves through the shock-layer, it undergoes deformation and gradually breaks up into smaller droplets while also evaporating due to its interaction with the surrounding fluid. This deformation and breakup of the droplet influence the subsequent dynamics of its impact, affecting the pressure distribution and overall damage inflicted. The mechanisms underlying droplet aerobreakup at high Mach numbers are intricate and still not fully comprehended.

Consensus among most researchers in this field revolves around classifying the process into distinct regimes, primarily based on the Weber number, denoted as We. Although researchers have studied aerobreakup mechanisms for many decades [1], there have been relatively few investigations conducted in the high Weber number regime. As a result, there is still no clear consensus on the dominant breakup mechanisms under these conditions, in particular, for high Mach numbers where phase change could be relevant.

The influence of phase change on these instability mechanisms and overall droplet aerobreakup process remains unexplored. Aluminum droplets exposed to shocks have been tested numerically [2] with sharp interface methods and phase change modeling, but the interface instabilities are not discussed nor present in their simulations, and empirical data for validation is absent. With these new set of experiments shown here from our co-authors, a much needed quantitative comparison not only of the shock-droplet interaction but also of the high-speed impingement has become available. The experiments have been performed at ambient conditions, around $M_S = 5$, obtaining realistic hypersonic

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post-shock conditions. Cloud dimensions, after-impingement jet speeds and reflected shock placements have been used to compare numerical and experimental runs.

Performing numerical simulations of shock-droplet interactions poses significant challenges, particularly at higher Mach numbers, due to the need for a numerical simulation approach that achieves a delicate balance between robustness and solution accuracy. Weighted Essentially Non-Oscillatory (WENO) schemes[3], employed in the current work, offer an appealing solution by effectively handling flow and material discontinuities, while enabling higher-order accuracy in smooth flow regions. In the case of multiphase problems, these schemes are commonly combined with flux schemes like the HLLC scheme utilized in this study, which more effectively capture gas/liquid interfaces. However, it is important to note that these schemes can also introduce numerical artifacts such as the carbuncle phenomena. Distinguishing these artifacts from interfacial instabilities requires careful interpretation and analysis of the results. Furthermore, there are limited algorithms available that can handle high Mach number flows while maintaining a high-order of accuracy, as the variable reconstruction and flux differentiation steps can lead to unbounded volume fractions, negative speeds of sound, or partial densities. To address this issue, the present study utilized a positivity-preserving limiters based on the work by Wong et al. [4], which not only mitigates the problem but also relaxes the requirements on the CFL number. The inclusion of phase change poses new challenges for the limiting procedures, and additional robustness steps are needed to preserve positivity and boundedness, specially at extreme temperature conditions and were previously tested in Refs. 5, 6.

While the main objective of the current research is to study droplet impingement, the history of the droplet needs to be taken into account as it is important for the impingement dynamics and is, therefore, an integral part of this study. Multiphase capabilities are the latest addition[5] to the in-house Cartesian Higher-Order Adaptive Multi-Physics Solver (CHAMPS) framework, which employs an Immersed Boundary Method (IBM) [7–10] to account for the geometry and Adaptive Mesh Refinement (AMR) to decrease the cost of the simulation based on chosen flow features. This newly developed simulation framework was used in this work to study droplet aerobreakup and impingement at high velocities following the experiments performed by Dworzanczyk et al. [11].

The current paper is organized as follows. It starts with a brief explanation of the governing equations in section III, the numerical setup and experiments in section II. The results section including comparisons with the experimental data is divided into three parts analyzing the shock structure around the moving droplet in section IV, the droplet aerobreakup phase in section V and the final droplet impingement phase in section VI. Finally, the paper closes with some general conclusions and a discussion on future steps in section VII.

II. Governing Equations

The Allaire [12] five-equation model has been used for this work, with the addition of the viscous terms and closed by the stiffened gas equation of state and basic homogeneous mixture rules. It consists of three mass conservation equations, one for each species, a momentum equation for each spatial dimension, an energy equation, and a non-conservative volume fraction advection equation. The governing equations are written in the form:

$$\frac{\partial \alpha_l \rho_l}{\partial t} + \nabla \cdot (\alpha_l \rho_l \mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial \alpha_{\nu} \rho_{\nu}}{\partial t} + \nabla \cdot (\alpha_{\nu} \rho_{\nu} \mathbf{u}) = 0, \tag{2}$$

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla \cdot \left(\alpha_g \rho_g \mathbf{u} \right) = 0, \tag{3}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u} \otimes \mathbf{u} + p\mathbf{I} - \mathbf{T}\right) = 0, \tag{4}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[(E+p) \mathbf{u} - \mathbf{T} \cdot \mathbf{u} \right] = 0, \tag{5}$$

$$\frac{\partial \alpha_l}{\partial t} + \mathbf{u} \cdot \nabla \alpha_l = 0. \tag{6}$$

$$\frac{\partial \alpha_{\nu}}{\partial t} + \mathbf{u} \cdot \nabla \alpha_{\nu} = 0. \tag{7}$$

T is the viscous stress tensor, which is given by

$$\mathbf{T} = 2\mu \left(\mathbf{D} - \frac{1}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right),\tag{8}$$

where μ is the molecular viscosity, which is calculated by following a simple mixture rule[13] given by

$$\mu = \alpha_l \mu_l + \alpha_v \mu_v + \alpha_g \mu_g. \tag{9}$$

In this work, all the parameters μ_l, μ_v and μ_g are assumed to be constant, and

$$\mathbf{D} = \frac{1}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right), \tag{10}$$

where the fluid phase is represented by the subscript k = l, v and g, referring to liquid, vapor and gas, respectively, α_k is the volume fraction occupied and ρ_k is the component density of either phase k, while ρ is the total local density. **u** is the local velocity vector, p is the static pressure, and $E = \rho (e + |\mathbf{u}|^2/2)$ is the total energy. Internal energy and pressure are related by the stiffened gas equation of state. The total density and mass fraction, volume fraction, and component density for either phase are related by

$$\rho Y_k = \alpha_k \rho_k,\tag{11}$$

where Y_k is the mass fraction. With this formulation, the volume fractions and mass fractions each add up to unity, i.e. $\alpha_l + \alpha_v + \alpha_g = 1$ and $Y_l + Y_v + Y_g = 1$. Equations (1)-(7) can also be written in vector form as

$$\partial_t \mathbf{W} + \partial_x \mathbf{F}^x \left(\mathbf{W} \right) + \partial_y \mathbf{F}^y \left(\mathbf{W} \right) + \partial_z \mathbf{F}^z \left(\mathbf{W} \right) + \partial_x \mathbf{F}^x_d \left(\mathbf{W} \right) + \partial_y \mathbf{F}^y_d \left(\mathbf{W} \right) + \partial_z \mathbf{F}^z_d \left(\mathbf{W} \right) + \Sigma \left(\mathbf{W}, \nabla \mathbf{W} \right) = 0, \tag{12}$$

where the state vector, the convective and viscous fluxes and source term are written as

$$\mathbf{W} = \begin{bmatrix} \alpha_{l}\rho_{l} \\ \alpha_{\nu}\rho_{\nu} \\ \alpha_{g}\rho_{g} \\ \rho u \\ \rho v \\ \rho w \\ E \\ \alpha_{l} \\ \alpha_{\nu} \end{bmatrix}, \quad \mathbf{F}^{x}\left(\mathbf{W}\right) = \begin{bmatrix} \alpha_{l}\rho_{l}u \\ \alpha_{\nu}\rho_{\nu}u \\ \alpha_{g}\rho_{g}u \\ \rho u^{2} + p \\ \rho v u \\ \rho w u \\ (E + p)u \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{F}^{y}\left(\mathbf{W}\right) = \begin{bmatrix} \alpha_{l}\rho_{l}v \\ \alpha_{\nu}\rho_{\nu}v \\ \alpha_{g}\rho_{g}v \\ \rho v u \\ \rho v^{2} + p \\ \rho w v \\ (E + p)v \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{F}^{z}\left(\mathbf{W}\right) = \begin{bmatrix} \alpha_{l}\rho_{l}w \\ \alpha_{\nu}\rho_{\nu}w \\ \alpha_{g}\rho_{g}w \\ \rho uw \\ \rho w w \\ \rho w^{2} + p \\ (E + p)w \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{\Sigma}\left(\mathbf{W}, \nabla \mathbf{W}\right) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$
(13)

In this formulation, the components of **W** are treated as conserved variables except for the volume fraction advection equation.

A. Phase change

With phase change, an additional source term is included on the right hand side of the Navier-Stokes equation, written as

$$\mathbf{S} = \begin{bmatrix} \frac{\rho}{\rho_I} \chi \left(g_g - g_I \right) \\ -\frac{\rho}{\rho_I} \chi \left(g_g - g_I \right) \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$
(15)

where $g_k = h_k - T_k s_k$ is the Gibbs free energy of phase k, and χ rate parameter of transition to phase equilibrium.

An algorithm developed by Chiapolino [14] is employed to obtain a solution assuming infinite fast relaxation rates. Validation of this approach can be found in the accompanying paper from Stoffel et al. [15].

B. Numerical Methods

A robust numerical method is employed to solve the governing equations. For spatial discretization, the fifth-order Weighted Compact Nonlinear Scheme (WCNS) from Ref. [4] and previously validated in Ref. [5] is used. The HLLC (Harten, Lax, and van Leer with Contact) flux scheme is implemented to accurately capture shock waves and contact discontinuities. For time integration, we adopt the third-order Strong Stability Preserving Runge-Kutta (SSPRK34) method. The Immersed Boundary Method (IBM) [16] with ghost cell filling is utilized to effectively handle the presence of solid boundaries.

III. Experimental Setup and Computational Setup

In order to allow for an efficient exploration of the different physics involved in droplet aerobreakup and impingement, it was decided to run the simulations assuming axisymmetry. The original experiment consists of a prismatic 4x4x6 inch projectile being shot at Mach 5 against droplets that levitate via an acoustic resonator. Details for the experimental setup can be found in the accompanying paper by Dworzanczyk et al. [17]. The computational domain extends over 25cm in x-direction and 30cm in radial direction. The droplets with diameters of 1.76mm and 1.91mm for the two runs are introduced upstream of the shock as illustrated in Figure 1b. A single droplet was spatially resolved with an equidistant grid spacing in x- and r-directions of $D/\Delta x=D/\Delta r = 310$. Figure 1a shows a snapshot of the droplet traversing through the shock layer where adaptive mesh refinement (AMR) is used to efficiently track the droplet, shock structure and resolve the boundary layer around the target geometry. [18] [19] Although the geometry cannot be replicated via an axisymmetric simulation, by choosing a diameter equal to the front face we were able to obtain very similar shock standoff distances. Two different speeds were chosen, 1640 m/s and 1808 m/s, based on two different shots performed in the experimental campaign. The data from the first shot will be used to study the droplet impingement phase. The reason that these two shots were chosen is that the first shot provided the clearest imaging data during the aerobreakup stage and the second shot during the impingement stage.

| <i>x</i> (<i>m</i>) | $\alpha_1 \rho_1 \ (kg/m^3)$ | $\alpha_2 \rho_2 (kg/m^3)$ | $\alpha_3 \rho_3 (kg/m^3)$ | u (m/s) | p(kPa) | α_1 | α_2 |
|-----------------------|------------------------------|----------------------------|----------------------------|-----------|--------|----------------------|--------------------|
| droplet | 1000 | 1×10^{-8} | 1×10^{-8} | 1640/1808 | 100 | $1-1 \times 10^{-8}$ | 1×10^{-8} |
| otherwise | 1×10^{-8} | 1×10^{-8} | 1.225 | 1640/1808 | 100 | 1×10^{-8} | 1×10^{-8} |

 Table 1
 Initial conditions for the droplet impingement simulation.

IV. Shock Structure Around Moving Droplet

Firstly, the shock structure formed around the moving droplet for simulations with different modeling fidelity are compared. The most notable difference in the shock structure can be observed behind the droplet, where the recompression shock is formed. Figures 2a-c show the experimental result on top and numerical schlieren on the bottom for the simulations with (a) inviscid without phase change, (b) inviscid with phase change and (c) viscous with phase change. For the inviscid simulation without phase change, the recompression shock appears to be disrupted by what



Fig. 1 (a) Simulation setup for the shock-droplet interaction case at Mach 5 and (b) instantaneous visualization of adapted mesh.

seems to be shocklets generated by the wake behind the droplet. The introduction of phase change appears to reduce the unsteadiness in the wake of the droplet and the recompression shock is more smooth similar to what is seen in the experiments.



Fig. 2 Numerical schlieren for (a) inviscid simulation without phase change, (b) inviscid simulation with phase change and (c) viscous simulation with phase change (bottom images) compared with images from experiments (top images) $15\mu s$ after crossing the shock.

Closely inspecting the inviscid run with phase change, it can be seen that the recompression shock still displays smaller wiggles while adding viscous terms removes wiggles completely similar to what is shown in the experiment. This result suggests that the wake dynamics are strongly affected by the presence of water vapor which reduces the unsteadiness in the wake. The effect of adding molecular viscosity is less severe but also reduces some of the unsteadiness. A comparison of the standoff distance of the shock upstream of the droplet reveals an overall reasonable agreement in the standoff distance for all three simulation approaches. The largest discrepancy arises for the inviscid simulation without phase change. A subtle difference between inviscid and viscous simulation with phase change can be observed. Inspecting the images from the simulations more carefully, it appears that, for the inviscid simulation

without phase change, the maximum vertical displacement is closer to what is seen in the experiment, but the shock immediately normal to the surface seems more flattened. It should also be noted that the increased standoff distance for this simulation suggests that the shape of the droplet is not captured correctly as the standoff is to first order driven by the size of the droplet. This observation may imply that it is not straightforward to extract the precise shape of the droplet from experimental images and the droplet appears much larger even in the front part of the droplet. This implies that, although figures 3 and 4 show how the radial extent seems to match more closely for the inviscid simulation without phase change, the distribution of the liquid phase is not correct for this case. When interpreting the radial displacement results in figure 4 it should be kept in mind that the radial displacement was measured as the furthest dark gray pixel in radial direction which is relying on the proper interpretation of these images and based on the gray-scale contrast provided.



Fig. 3 Image from experiments overlaid with water massfraction contours from simulations 15 μ s after the droplet has crossed the shock. Green, blue and red lines refer to inviscid simulations with and without phase change and viscous simulation with phase change, respectively.

V. Droplet Aerobreakup

Water droplet aerobreakup mechanisms have been studied in some detail at lower speeds [1, 20, 21] and it has been pointed out in various studies that phase change does not play an important role in the breakup process. [22] Experiments are typically performed in shock tubes considering relatively cold flow [1], which greatly underestimates temperature or enthalpy conditions attained in free flight. The range of temperatures reached by the reflected shock traveling with the droplet is 2700-3300 K for this numerical experiment, so phase change is expected to be playing an important role. Moreover, at those temperatures water starts dissociating, nonetheless, this type of chemistry is still not accounted for in this effort. This work serves as a first step towards modeling phase change as part of the liquid droplet demise. In figure 3, a comparison between the mist or "cloud" the droplet turns into after traveling 15 μs inside the shock layer is presented. To reduce numerical diffusion artifacts, the outer contour is defined by selecting a 5% water mass fraction contour for all cases. For the inviscid simulation without phase change, the water mass fraction is equal to the liquid mass fraction alone, but in the cases with phase change, it is the sum of both vapor and liquid mass fractions.

The inviscid and viscous simulations with phase change closely resemble each other, with the viscous case showing a wider water region after the front face and before the wake. The simulation without phase change is very different, and spatially it looks much closer to the experiment, but this could be misleading considering the previous comments about the interpretation of the images from experiment. In order to capture the instabilities driving the wake dynamics and the appearance of the gray cloud in the images the simulations would need to be performed fully 3-D, while the current simulations are axisymmetric, thus, neglecting relevant physics. Three-dimensional droplet aerobreakup simulations, albeit disregarding phase change, have been performed with CHAMPS and analyzed in detail in a prior conference paper [23]. In these simulations, we match the vertical deformation of the droplet much better, although a slight overprediction was observed pointing us in the right direction when interpreting the current axisymmetric results.

Turning the attention back to the radial displacements provided in figure 4a, an additional simulation was performed where the initial circular droplet was changed to an ellipsoid, as the experiments were not showing a perfectly spherical shape. Right away it can be spotted how the ellipsoid shape does not help capturing the right deformation (pink symbols), so it must have to be related to the instabilities and successive turbulent wake formation. Both experiments and simulations show there are instants at which the droplet deforms much faster, followed by a plateau. This is indicative of the more violent bursts originating from the front face of the main body of water. Those bursts are strongly suppressed when the phase change is activated, but they are still present. Those plateau regions differ for all the numerical experiments, meaning the instabilities are strongly affected by droplet shape, viscosity and addition of phase change. Adding molecular viscosity seems to maintain the tendency of the droplet size to continuously grow, tendency which is supported by the experiments. The results for the horizontal trail length in figure 4b more closely agree with the experiments for all cases except the simulation without phase change being the main outlier in the data. Finally, it is hard to delimit the horizontal droplet deformation as from the experiments is difficult to identify the liquid water phase due to the presence of large amounts of water vapor around the droplet.



Fig. 4 (a) Maximum vertical deformation, and (b) maximum length of the horizontal trail from the front face of the droplet for different simulations and experiment.

To closer inspect the droplet aerobreakup process a close-up of the droplet for the simulation without phase change liquid water volume fractions for simulations without phase change and water vapor volume fractions for simulations with phase change at two time instants at $2\mu s$ and $10\mu s$ after crossing the shock are shown in figure 5. Development of the interfacial instability on the front of the droplet and shear-layer instabilities around the edges and wake of the droplet are clearly visible. The interfacial instability seems to be suppressed by the presence of water vapor which is in agreement with what appears to be happening in the experiment. The development of the shear layer instability is also strongly affected by including phase change. The shedding is affected both in terms of the wavelength and strength of the vortical structures that can be observed in the visualization. Inspecting the movies taken in the experiment, at the early stage the shedding is subtle, which leads us to believe that our simulations with phase change more correctly predict the ongoing physics.

The frequency of the bursts is also a sign that the shear-layer instabilities from the vapor layer might be dominating the formation of the vapor cloud shape. The current results are clearly not fully conclusive, as again, it needs be pointed out that including 3-D effects will change the wake dynamics dramatically. 3-D simulations with phase change are currently underway. Our previous no-phase change simulations [23] have shown ring-like shedding patterns from the front face that look very similar to the ones observed in the experiments for cold flow experiments. Further investigations are clearly needed, but the current simulations suggest a vapor layer may be important to capture the physics properly. The width of this layer is spurious as it is smeared out by the numerics as well as the infinite relaxation time contribute to modeling errors, and the combination could lead to this overprediction. Grid convergence studies show some sensitivity of this vapor layer width to the refinement, but not a direct correlation. Aluminum droplet simulations from an accompanying paper by Stoffel et al.[15] show a more deformed front face when leaving the droplet static and moving the shock.



Fig. 5 (a,c) Liquid water volume fractions for simulations without phase change and (b,d) water vapor volume fractions for simulations with phase change at two time instants at (a,b) $2\mu s$ and (c,d) $10\mu s$ after the droplet has crossed the shock.

VI. Impingement

Initially, one of the key challenges to perform this research was to maintain a stable simulation as the droplet is impinging at ultra-high velocities. The high speeds at which the droplet hits the wall cause pressures in the order of GPa at the moment of impact, as well as the creation of shock waves inside the droplet that cause the droplet to stretch as the shock travels through the droplet, gets reflected back and forth inside. The stiffened gas p_{inf} parameter is in the order of 1 GPa, but once the negative pressures that form inside the droplet exceed that (absolute) value, there is a need to limit the solution or the speed of sound will become negative. Doing this is in a way that is unphysical will lead to numerical blow-up eventually. Hence, in order to provide a physical solution, we need to use a thermochemical relaxation procedure detailed above to properly model the physics causing the stretching of the water droplet.

The thermochemical relaxation model that is currently being employed to account for the phase change assumes an infinitely fast relaxation rate, meaning that the mixture is always going to be at equilibrium by the end of each update step. This allows us to run the these simulations parameter-free, which is very convenient, but in reality this is likely not accurate, especially at the very energetic early stage of the impingement, when, due to the very high temperatures attained, some non-equilibrium effects need to be accounted for. It seems to be a reasonable starting assumption nonetheless if considering the entire process from start to end, as the flow will always end up as an admissible physical mixture, and the extreme conditions are seen only over a very short relative time period. Our equation of state is also flawed in that respect, as transcritical or supercritical effects of the water are not being properly considered [24]. Negative pressures are never reached with the current simulation approach, meaning the droplet is not allowed to stretch significantly before undergoing cavitation. Mass fraction plots show the evolution of the water droplet after impact in figure 6.

The jet formed in the radial direction covers almost 4 mm in $1\mu s$, but after $5\mu s$ have passed since impingement, it has only traveled 10 mm. The initial speed at which it is moving seems to slow down due to viscous interactions with the wall, and subsequent appearance of complex instabilities arising from the liquid and vapor layer sheets. The formation of an interfacial fingering structure starts to emerge at $2\mu s$ which has some similarity to what is observed in the experiments. The different snapshots of liquid water and water vapor mass fraction contours illustrate how quickly the liquid water phase is converted to water vapor, albeit the core of the droplet is still dominated by the liquid phase. Towards the end of the impingement phase the liquid phase is concentrated toward the edges of the gas-liquid water cloud for times greater than $5\mu s$.





Fig. 6 Comparison of water mass fraction Y_w (top row), liquid mass fraction Y_l (middle row) and vapor mass fraction Y_v (bottom row) at different times after droplet impingement for the viscous simulation with phase change.

By activating phase change the impingement simulation can be run robustly, and the resulting shocks and flow structures that arise from the collision can be analyzed for the first time in numerical simulations. The water vapor formation process in the post-impingement stage is visualized in figure 7, which was created using the same approach used before to compare the aerobreakup shapes by visualizing the $Y_w = 5\%$ contours. A comparison of numerical schlieren computation is also presented to illustrate the effect of viscosity after impact. A slight overprediction of the gas-liquid water phase is present in both the inviscid and viscous simulations. In order to obtain a time-accurate representation, the exact time was counted since the instant at which the droplet touches the wall, both in the experiments and computations. From the experiments, it is not straightforward to determine the exact time of impingement due to because, due to imaging artifacts, the location of the wall cannot perfectly be detected. There is certainly a mismatch in the upcoming recompression shocks from the back of the droplet which can be explained by minor differences in the shock standoff distance of the incoming droplet.

The characteristic of the shock created by the impact of the droplet are not in good agreement between the experiments and the simulations which cannot be explained by slight differences in the standoff distance as both simulations have been synchronized through the impact time. Figure 8 provides a qualitative comparison intended to show how the shapes of the reflectd shocks from the experiment and simulation look side by side. The shock front looks very similar, and the presence of shocklets inside the region behind the shock front and the wall can be seen both in the experiments and numerical experiments, but the structures observed in the simulations remain much stronger. This could be explained by the inability of the current algorithm to physically deal with very high temperature phase change, and dense liquid mass ejected still carrying strong shocks. The mismatch in the recompression shock could also be related to the AMR releasing the finest grid level around this feature. Another explanation is that 3-D effects may be important as well. The front-shock flattening in the normal direction is captured, and the outer shock layer is revealed to be formed by the merging of distinct shocks, not being perfectly smooth. The inviscid simulation has some limitations, which can clearly be observed in figure 7, as the slip boundary condition fails to decelerate the vertical liquid jet, resulting in a spurious liquid layer very close to the surface, pictured in blue. It is also worth noting that some of the transport properties are assumed to be constant and homogenous mixture rules are applied to obtain mixture properties. This is still a crude approach and the influence of temperature-dependent parameters as well as different mixing rules will be explored in the future.



Fig. 7 (a) Water mass fraction of $Y_w = 5\%$ contour lines for the inviscid (blue) and viscous (red) simulations, at 2.75 μ s after impact. (b) Numerical schlieren comparison of the viscous case (left) and the inviscid (right).



Fig. 8 Comparison of experimental image (left) and numerical schlieren (right) at $4\mu s$ after impact.

A quantitative comparison of the vertical and horizontal jet speeds are provided in figures 9a and 9b. The plot of the vertical position of the water in figure 9a seems to confirm the spurious behavior of the inviscid simulations where the jet speed is severely overpredicted. Comparing the vertical jet position for the viscous simulation against the experiment a mean difference of around 30% is apparent, and, for the horizontal position, the average difference is around 40%. Coincidentally, when initializing our droplet to thermochemical equilibrium, there is an overprediction of 38.4% in water density. The error in density translates to a similar magnitude in error for the kinetic energy that the droplet carries, and serves as a possible explanation for the observed discrepancies. Improved equations of state are available in the literature [24, 25], but the positivity-preserving proofs that our higher-order numerical scheme relies on are not readily derived, so questions about sufficient robustness using more complex equations of state need to be addressed. Efforts to overcome this issue are currently underway and to allow for the use of more advanced equations of state in future investigations.



Fig. 9 (a) Vertical and (b) horizontal post-impingement water jet position versus time.

VII. Conclusion and Future Steps

Numerical simulations of droplet impingement at high velocities have been performed considering different degrees of modeling fidelity and the results were compared against recent experiments conducted at the Southwest Research Institute. First and foremost, the numerical simulations do not perfectly agree with experiments, but the newly developed framework to perform robust and time-accurate simulations over the entire duration of droplet aerobreakup and impingement phases has been established. The inaccuracies in the predictions are not unexpected due to the complex multiphase physics that are at play. In the future to obtain closer agreement between the simulations and experiments, we will be including more complex equations of state and address some of the numerical stability concerns that may come with it. Using more advanced equations of state will solve the density discrepancies which could be the key to match more closely the post-impingement features observed in the experiment. Enhancing the non-equilibrium phase change capabilities and supercritical state modeling will also rely on having the improved equation of state available. Finally, three-dimensional simulations are currently performed to address some of the concerns about more accurately capturing the characteristics of the wake dynamics.

Acknowledgments

Funding support by the Office of Naval Research under contracts N00014-22-1-2443 with Dr. Eric Marineau as program manager is gratefully acknowledged. The authors would also like to thank the University of Maryland for their Juggernaut and Zaratan computing resources, as well as NASA for their Pleiades supercomputer. Support from our collaborators Tyler Stoffel and Savio Poovathingal has been essential to develop the phase change algorithm.

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