Numerical modeling of atomization in compressible flow

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Numerical modeling of atomization in compressible flow

by

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DEDICATION

To my family.
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ABSTRACT

The study of atomization in supersonic combustors is critical in designing efficient and high performance scramjets and ensuring reliable ignition in their complex startup conditions. Numerical methods incorporating surface tension effects have largely focused on the incompressible regime as most atomization applications occur at low Mach numbers. Simulating surface tension effects in compressible flow requires robust numerical methods that can handle discontinuities caused by both material interfaces and shocks. In this work, a shock and interface capturing finite volume scheme is developed to solve the compressible multicomponent Navier-Stokes equations with capillary forces. Shock capturing is performed with a Harten-Lax-van Leer-Contact (HLLC) Riemann solver modified to account for the surface tension induced pressure jump across the gas-liquid interface. Interface capturing is performed with a diffuse interface model. The solver utilizes a total variation diminishing (TVD) third-order accurate Runge-Kutta method for time-marching and second-order accurate TVD spatial reconstruction. To prevent numerical smearing of the material interface, an interface compression/sharpening scheme is required. A PDE-based compression scheme is implemented and with developments to account for surface tension effects. The approach is successfully used to model liquid atomization problems but is not discretely conservative. To address this, a Tangent of Hyperbola for INterface Capturing (THINC) interface reconstruction scheme is investigated with developments to account for the phasic densities in the context of the five equation model. The resulting solver can account for the effects of compressibility, surface tension, and molecular diffusion in interfacial flows. One and two-dimensional benchmark problems demonstrate the desirable interface sharpening and conservation properties of the approach. Two and three-dimensional examples of primary atomization of a liquid jet in a Mach 2 crossflow and secondary atomization of a liquid droplet after its interaction with a shockwave demonstrate the robustness of the method. The dependence of Weber and Mach number on the breakup characteristics
of cylindrical liquid columns are then investigated with a series of numerical experiments. A range of Weber numbers is considered for two different shock-droplet interactions consisting of either subsonic or supersonic post-shock conditions. In the subsonic case, a number of different breakup modes are observed with a strong dependence on the Weber number and provide good correlation with experimental observations. Droplets at lower Weber numbers exhibit lower drag coefficients with implications for point particle type atomization models. In the supersonic case, less variation of the drag coefficient as a function of Weber number is observed.
CHAPTER 1. INTRODUCTION

The current research is motivated by the importance of fuel atomization in high-speed propulsion systems, particularly supersonic combustion ramjets, or scramjets. Scramjets are facing renewed interest as a result of the successful USAF X-51 scramjet flight testing and potential ramifications of hypersonic missiles and space launch vehicles [1]. Unlike ramjets which operate with subsonic air in the combustion chamber, scramjets contain supersonic flow throughout the engine. The complexities involved with supersonic combustion meant the first successful scramjet flight test occurred over 30 years after the initial conception of the engine [2]. Efficient combustion is greatly dictated by the fuel-injection scheme but there is a limited understanding of the effect of design parameters on the atomization process [3]. Additionally, due to the high flow speeds, fuel residence times are very short. This means the fuel must be rapidly mixed and efficiently burned before it is expelled from the engine but without causing engine unstart due to combustion related pressure rises [4]. As scramjets operate at high speeds, they require alternate means to initially fly. For example, the X-51 was carried on a B-52 aircraft before being released and accelerated by a solid rocket booster to Mach 4.5 before the scramjet engine was ignited [5]. Such conditions are difficult to replicate experimentally making numerical modeling of the complex flow conditions experienced during engine startup and hypersonic flight all the more important. To this end, the ultimate goal of the present research is Computational Fluid Dynamics (CFD) modeling of liquid atomization in supersonic crossflows, including the effects of capillary and viscous forces. This includes isolated droplet-shock interactions (secondary atomization) and liquid jets in crossflows (primary atomization) so as to better understand the physical mechanisms occurring in a hypersonic vehicle during engine startup and flight.
While significant effort has been invested into investigations of primary and secondary atomization of liquids in incompressible flows (see [6, 7] for recent reviews), the effects of surface tension in high speed compressible flows has not yet been investigated numerically in any significant detail, perhaps in part because accurately modeling surface tension effects in compressible multiphase flows is incredibly challenging. The multiphase nature of the flow requires an adequate description of the interface between the gas and liquid and capturing the interfacial dynamics (i.e. surface tension) in the presence of large density ratios and strong shocks requires a robust numerical scheme. To preserve the physical nature of the flow the gas-liquid interface should remain sharp, however, a sharp interface introduces difficulties in accurately calculating the interface curvature on which the capillary force is derived. Maintaining a sharp interface also requires competing with the numerical dissipation introduced by shock-capturing schemes to handle discontinuities. The efficiency of the numerical scheme is also highly important because simulating the full dynamics of liquid atomization requires good spatial and temporal resolution over long simulation times.

A finite volume method that addresses a number of these challenges has been developed and can be used to efficiently simulate liquid atomization in supersonic crossflows. First, a summary of the current state-of-the-art will be given in the following sections. This will include an overview of surface tension modeling in compressible frameworks and CFD methods for multicomponent flows. This will be followed by sections on the important non-dimensional parameters in the presence of capillary and viscous forces and finally, the layout of the remaining chapters in the thesis.

1.1 Numerical atomization modeling

The simulation of atomization in supersonic flows is the ultimate goal of the present research. This includes both primary and secondary atomization. Primary atomization is represented by the initial breakup of a liquid sheet or jet into smaller drops or filaments, for example, a liquid jet in a crossflow. Droplets formed during primary atomization can further deform and breakup in a process known as secondary atomization. Such conditions occur in the case of a shock wave impacting a droplet, or shock-droplet interaction. While liquid jets [8, 9, 10,
11, 12, 13, 14] and the early stages of droplet breakup [15, 16] in supersonic conditions have been studied numerically in the past, surface tension has largely been neglected. Designers commonly employ empirical atomization models which give the droplet size distribution in terms of the dimensionless Reynolds, Weber, or Ohnesorge numbers via empirical relationships derived from experimental measurements [3]. These dimensionless numbers are important because they relate the viscous and surface tension forces to the inertial ones. In terms of atomization, the deformation due to the aerodynamic forces is resisted by the viscous and surface tension forces [6]. Numerical simulations of the atomization process can provide deeper insight into the physical mechanisms of atomization and the impact of flow parameters on droplet breakup.

As most applications of atomization occur at low Mach numbers [17], numerical modeling has largely focused on the incompressible regime [18, 19, 20, 21]. Accordingly, surface tension has been studied in a wide variety of incompressible atomization applications such as fuel sprays, agricultural systems, liquid metal fabrication, and printing processes to name a few. This was largely made possible by the development of the Continuum Surface Force (CSF) method [22] which incorporates the interfacial surface tension force into the fluid governing equations as a volume force.

Interestingly, while the CSF method was developed almost 25 years ago, only relatively recently has surface tension been incorporated into a compressible framework where it remains a challenging problem. Numerical simulations of atomization in this flow regime thus far have focused on the early stages of droplet breakup where surface tension effects are not expected to play a significant role [15, 16]. Meanwhile, existing compressible models with capillary effects have focused on low Mach number applications for which compressibility effects are important, such as evaporation, cryogenics, cavitation, or bubble collapse near a wall [23]. A brief summary of the existing compressible flow models which incorporate surface tension effects follows.

Perigaud and Saurel developed a compressible flow model with capillary effects by applying the CSF model to the compressible Navier-Stokes equations in the context of the five equation model, a simplified form of the Baer-Nunziato equations [23]. The Baer-Nunziato non-equilibrium seven equation model yields separate mass, momentum, and energy conservation
equations for each phase. The five equation model assumes pressure and velocity equilibrium between the phases such that a single momentum and energy equation is solved for the mixture. Including individual mass conservation equations for each phase plus a level-set equation to track the interface gives five equations total. The surface tension force is incorporated into the governing equations in a conservative fashion based on terms developed for incompressible flow modeling with surface tension [18]. An exact Riemann solver developed for the Euler equations was modified to account for the pressure jump due to surface tension across the contact discontinuity. The use of an exact Riemann solver avoids the issue of the numerical smearing of the interface despite the interface being modeled using the Diffuse Interface Method (DIM). But, a diffusive approximate Riemann solver is employed for the first few timesteps of each simulation to slightly smear the interface and allow more accurate curvature computation before switching to the exact Riemann solver. The model was applied to several low Mach number test cases. These included a static drop in equilibrium, an oscillating droplet, falling droplet breakup due to gravity effects, the rise of a bubble in liquid, bubble explosion near a solid wall, and colliding droplets. As it turns out, there is a general lack of high Mach number validation problems for flows with surface tension effects.

Chung derived a theoretical two-dimensional model for simulating bubbly gas liquid flows with surface tension and compressibility effects [24]. The model uses the Baer-Nunziato non-equilibrium equations such that there are separate equations for the momentum and energy in each phase. However, perfectly spherical bubbles are assumed (i.e. deformation is not accounted for in curvature computation) and it was apparently never developed into a working numerical model.

Braconnier and Nkonga developed a methodology to simulate compressibility effects in flows with surface tension using a linearized relaxation Riemann solver and a low Mach preconditioner [25]. However, as with Perigaud and Saurel, only low Mach number flows with surface tension were considered. The method was shown to accurately simulate shock-bubble (gas-gas) interactions in air without the effects of surface tension while an oscillating droplet and a falling water drop in air were used to verify the surface tension effects. No comment was made on the ability of the method to simulate gas-liquid shock-droplet interactions with the effects of
surface tension, and it is not clear if the relaxation scheme employed would be efficient in such simulations.

Nguyen et al. [26] developed a discontinuous Galerkin Arbitrary Lagrangian Eulerian (ALE) based method for compressible flows with surface tension. The gas-liquid interface is explicitly tracked with a deforming unstructured mesh. The mesh nodes corresponding to the interface are moved with the local flow velocity. This mesh motion is accounted for in the numerical fluxes which are determined from an exact Riemann solver with modifications to account for the surface tension induced pressure jump across the interface. Local remeshing in the form of node addition, deletion, or edge flipping is performed if the mesh quality overly deteriorates due to the interface motion. This type of interface tracking constitutes a Sharp Interface Method (SIM) as the properties of the fluids can be totally discontinuous across the interface. The method was applied to a static droplet test and several oscillating ellipse cases.

Shukla [27] presented results of a falling droplet in air under the effects of surface tension, however only very limited information is summarized on how the surface tension effects were incorporated beyond statements that curvature was computed using standard second order central differences together with the associated conservative fluxes of [23] to account for capillary forces. But, the paper demonstrated the feasibility of an interface compression technique in countering the numerical diffusion of the interface when using a DIM. As a result, the immiscibility of the fluids are well preserved and the gas-liquid interface is well defined. This is an important characteristic which will be revisited in later sections.

Nguyen and Dumbser developed a compressible model with surface tension effects incorporated in non-conservative form using a path-conservative discretization of the source terms and the DIM [28]. The non-equilibrium Baer-Nunziato system is assumed while specific Osher, Rusanov, and Roe-type solvers were developed to account for surface tension terms. They showed their specific discretization was well-balanced, meaning that for a steady bubble in equilibrium with exact curvature prescribed, the model satisfies the Young-Laplace law (surface tension induced pressure jump) exactly. The feasibility of the method was validated with one-dimensional examples with constant prescribed curvature. Two dimensional applications
were also limited to low Mach number flows with static and oscillating droplet tests and a falling liquid droplet in air.

Fechter and Munz [29] developed a three-dimensional discontinuous Galerkin SIM based solver for simulating compressible flows with surface tension and phase change. The interface is resolved using the ghost fluid approach with a local Riemann solver that accounts for both surface tension and phase change effects. The interface curvature computation is improved using local subcell refinement near the interface which is separately solved using a second order finite volume TVD scheme. The method is applied to static and oscillating ellipse droplet tests including surface tension and phase change (evaporation). It is also applied to shock-droplet interaction simulations but in the absence of surface tension.

Schmidmayer et al. [30] developed a numerical model and method for simulating compressible flows with capillary effects. A conservative form of the surface tension force is used together with a DIM approach. The method was successfully applied to a shock-droplet interaction problem but did not utilize an interface sharpening scheme and as a result showed significant diffusion of the gas-liquid interface.

Bo et al. [31] developed a front-tracking ghost fluid framework for studying the primary breakup of a liquid jet injected into a quiescent high-pressure gas. The droplet size distribution of the simulation agrees well with a log normal fit with a significant number of droplets of different sizes produced.

Chang et al. [32] developed a front-tracking method for performing direct numerical simulations of interface instabilities with high gas-liquid density and viscosity ratios and surface tension forces. The paper includes a wide array of test problems and provides brief summaries of prior work on the topics. It utilizes an adaptive mesh refinement scheme to resolve the boundary layer on the droplet surface up to an astonishing $D/800$ grid resolution. The droplet studies are performed using a 3D-axisymmetric solution domain and resolve intricate interfacial instabilities during the droplet deformation process.

Xiao et al. [33] performed Large Eddy Simulations (LES) of the primary breakup of a liquid jet in supersonic crossflows at various Weber numbers. They utilized a coupled level set/volume of fluid approach to track the interface with an incompressible solver for the liquid
phase and a compressible solver for the gas phase. This was achieved via independent evolution of the coupled gas and liquid phases through specification of distinct boundary conditions at the gas-liquid interface.

Two other studies mentioned for completeness are the relaxation Riemann solver of Rohde and Zeiler [34] and the sharp conservative interface method of Luo et al. [35]. Rohde’s method incorporates surface tension and phase change into the Riemann solver but was only applied to one dimensional spherically symmetric problems, with the emphasis being on evaporation effects. Luo et al. developed an incompressible solver but used a weakly compressible formulation with surface tension effects incorporated into a non-iterative linearized Riemann solver. This was combined with an interface reconstruction technique to treat the interface using the SIM.

This concludes the survey of compressible flow models with surface tension. Many of these involve surface tension in compressible but low Mach number applications. Only the recent study of Xiao et al. [33] directly addresses the primary objective of this work which is directly simulating the injection of a liquid jet into a supersonic crossflow. This is due to the difficulties associated with modeling the atomization conditions inside a scramjet which requires a compressible methodology capable of handling strong shocks and high density ratios with the presence of surface tension forces. While the above mentioned studies provide clues as to how this may be achieved, there is no clear path defined in the literature towards such simulations.

### 1.2 Compressible multicomponent flows

An integral part of the simulation of multicomponent flows is the treatment of the interface. Such treatment can be broadly categorized as either a Sharp Interface Method (SIM) or a Diffuse Interface Method (DIM). Both the SIM and the DIM approaches have been employed in the previously mentioned models with surface tension. A brief review of these two approaches follows.
1.2.1 Sharp Interface Method (SIM) approaches

Interface tracking methods fall under the SIM umbrella whereby the fluid properties across the interface can be naturally treated in a discontinuous way. There are a number of different varieties of interface tracking methods. Arbitrary Lagrangian Eulerian (ALE) methods involve a mesh that deforms with the interface [26, 29, 36, 37, 38]. This generally requires the use of unstructured meshes and potentially computationally complex remeshing algorithms. A similar approach is the free Lagrange method [39, 40, 41] which behaves as an unstructured mesh but with connectivity that can freely change as the mesh nodes move.

Front tracking methods [42, 43, 44, 45, 46, 47] utilize a fixed grid but separately track a front (the interface) and make appropriate modifications to cells through which the front crosses to account for the discontinuity. Such modifications can result in excessively small grid cells which can negatively affect numerical stability without special treatment. Also, large topological changes can be difficult to handle.

Ghost fluid and level set methods [48, 49, 50, 51, 52, 53] involve defining a band of cells near the interface for which a fluid mixture or ghost fluid exists. The interface discontinuity can be preserved by discarding the ghost fluid state on one side of the interface [53] or a level set reinitialization technique [54].

1.2.2 Diffuse Interface Method (DIM) approaches

The present research instead utilizes an interface capturing method [55, 56, 57]. The method is analogous to the concept of shock capturing inherent in compressible flow algorithms and can easily handle large topology changes in the interface. The method adds an additional conservation equation to capture the fluid interface, is simple to implement in multiple dimensions, and can be accurately used to simulate complex interfaces with fixed Cartesian grids. However, the main drawback of the approach is numerical smearing of the material interface, which in the presence of large density ratios and strong shocks can generate significant errors in computations of shock-interface interactions of otherwise immiscible fluids [27, 58].
There are several available approaches to counter the numerical diffusion of the interface. One option is the use of high resolution Weighted Essentially Non-Oscillatory (WENO) schemes [59, 60] for reconstruction of the solution variables. The method has been shown to accurately capture material interfaces with minimal numerical diffusion and has been successfully used to simulate the early stages of droplet breakup [16], however, the non-TVD (Total Variation Diminishing) nature of the WENO reconstruction may not ensure positivity of volume fractions and could cause difficulties in computation of interface curvature, a required parameter for incorporating surface tension. Additionally over long timescales this method will also succumb to excessive numerical diffusion of the interface.

To guarantee TVD solutions that are well-bounded, a second order flux reconstruction with flux limiting can be used. In this case, numerical diffusion can quickly deteriorate the interface such that additional steps must be taken to counter such behaviour. One option is to employ a corrective “post-processing” step after every physical timestep such that the numerical diffusion is reversed using either an anti-diffusion or compression technique. So et al. developed such an anti-diffusion method for incompressible flows [61] and later extended it to compressible flows [62]. The key idea is that an anti-diffusion equation is solved based on the specific numerical diffusion properties of the advected volume fraction equation and numerical scheme employed. The associated anti-diffusion fluxes are then applied to the conservative equations in a thermodynamically consistent and conservative manner so that the material interface remains sharp throughout the entirety of the simulation. An advantage of the method is that no interface normals or curvature terms need to be computed, however, it was not applied to simulations with strong shocks or large density ratios, and so it is not clear how well it would behave in such situations. Additionally, the approach is specific to the diffusive properties of the discretization scheme employed.

A more general approach is the interface compression method of Shukla et al. [58] with recent extensions by Tiwari et al. [63]. It was shown to accurately sharpen the interface during shock-interface interaction in the presence of high density ratios and strong shocks despite being discretely non-conservative. The method is based on concepts originally developed for the conservative level set method in incompressible flows [54, 64, 65]. However, the nature
of compressible flow (and shock waves) means large density gradients may not be tied to the material interface and thus the extension from the conservative incompressible version is not straightforward.

A conservative reconstruction based interface sharpening approach is the THINC (Tangent of Hyperbola for INterface Capturing) method [66]. The approach uses the hyperbolic tangent function to reconstruct the solution variables in the vicinity of the interface and unlike the interface compression schemes described above, does not require modifications to the governing equations.

Further details of the interface compression and THINC approaches are left for later chapters. Specifically, Chapter 2 includes further investigations of the interface compression approach with developments to account for surface tension. Meanwhile Chapter 3 compares the interface compression approach to the THINC scheme which has been further developed in this thesis to a general density based compressible formulation.

1.2.3 Summary

Generally, SIM approaches handle discontinuities in a natural way. However, they are not always well suited to large interface deformations and can involve geometrically complex reconstructions, remeshing, or require special thermodynamic treatment at interfaces. The DIM is straightforward to implement in multiple dimensions and easily handles complex topological changes in the interface, however, depending on the nature of the Riemann solver employed the interface can become overly diffused leading to significant error, especially in the presence of strong shocks and high flow speeds. For the sake of efficiency and robustness the use of diffusive non-iterative approximate Riemann solvers in conjunction with an interface sharpening algorithm to prevent numerical smearing of the interface is preferred.

1.3 Non-dimensional parameters and atomization modes

In compressible gas/liquid two fluid flows the following parameters can be defined:

- $N = \mu_l/\mu_g$ - viscosity ratio of liquid to gas.
• \( \epsilon = \rho_l / \rho_g \) - density ratio of liquid to gas.

• \( \text{Re} = \frac{\rho_g u l}{\mu_g} \) - Reynolds number - ratio of inertial to viscous forces.

• \( \text{We} = \frac{\rho_g u^2 l}{\sigma} \) - Weber number - ratio of inertial to surface tension forces.

• \( \text{Oh} = \frac{\mu_l}{\sqrt{\rho_g l \sigma}} \) - Ohnesorge number - ratio of viscous forces to inertial and surface tension forces.

• \( M = u / c \) - Mach number - ratio of velocity to acoustic speed.

Generally the length scale \( l \) is taken as the droplet or jet diameter and the velocity \( u \) is the relative velocity between the gas the liquid. Note that the Reynolds and Weber numbers are related through the other parameters as follows:

\[
\text{Re} = \sqrt{\frac{\text{We} \cdot N}{\epsilon \cdot \text{Oh}}}.
\] (1.1)

For air-water droplet simulations \( \epsilon \sim 1000, \ N \sim 45 \). For validation purposes, we are interested in atomization behaviour for \( \text{Oh} < 0.1 \) since the discrepancy between secondary breakup modes in that regime remains relatively constant [6]. A plot of the relationship between the Weber and Reynolds numbers as a function of the Ohnesorge number is given in Fig. 1.1. It should be noted that for \( \text{Oh} \sim 0.1 \), the Reynolds number is approximately the same order of magnitude as the Weber number. This can be significant when using an explicit time-stepping scheme, as for numerical stability the diffusion number is highly restrictive.

For \( \text{Oh} < 0.1 \), these breakup modes are summarized in Table 1.3 from [6]. Reproducing the behavior of and transition between these regimes is a good exercise for atomization validation. But it is important to note that the number of droplets produced generally increases while the droplet size decreases with increasing Weber numbers. As a result, adequate resolution of the multiple scales involved in simulations with high Weber numbers means higher computational requirements exist than for similar simulations at lower Weber numbers. Finally, while these breakup regimes are described for secondary atomization of a liquid droplet, similar breakup regimes exist for the primary atomization of liquid jets [7].
Figure 1.1  Reynolds number vs. Weber number at different Oh numbers.

Table 1.1  Atomization modes as a function of Weber number for Oh < 0.1 [6].

<table>
<thead>
<tr>
<th>Mode</th>
<th>We Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vibrational</td>
<td>0 &lt; We ∼ 11</td>
</tr>
<tr>
<td>Bag</td>
<td>∼ 11 &lt; We ∼ 35</td>
</tr>
<tr>
<td>Multimode/Bag-and-stamen</td>
<td>∼ 35 &lt; We ∼ 80</td>
</tr>
<tr>
<td>Sheet-thinning</td>
<td>∼ 80 &lt; We ∼ 350</td>
</tr>
<tr>
<td>Catastrophic</td>
<td>We ∼ 350</td>
</tr>
</tbody>
</table>
There also exists a non-dimensional characteristic breakup time $T$ defined as \cite{67, 68}

$$T = t \frac{u}{\sqrt{\epsilon l}}$$

(1.2)

where $u$ and $l$ are defined as above. Such a timescale is commonly used to non-dimensionalize atomization simulations.

Finally, this thesis is primarily focused on the development of a numerical approach to simulate atomization in compressible flows. While some of the physics of atomization are investigated for validation and demonstration purposes, interested readers can refer to recent and thorough reviews by Broumand and Birouk \cite{7} for primary atomization and Guildenbecher et al. \cite{6} for secondary atomization.

### 1.4 Thesis organization

This thesis outlines the development and initial applications of a finite volume method for simulating compressible interfacial flows with (or without) the presence of surface tension and molecular diffusion effects. Chapters 2 and 3 are manuscripts submitted to the Journal of Computational Physics. Chapter 2 presents the initial model development, including extensions of an HLLC Riemann solver and interface compression scheme to account for the surface tension induced pressure jump across the gas-liquid interface. If the exact interface curvature is prescribed, the surface tension induced pressure jump is captured by the model to within machine precision. A simple approach for numerically computing the curvature within the diffused interface region is also developed. However, the employed compression scheme is discretely non-conservative and possesses significant resolution requirements to properly resolve fine-scale interfacial features. To address this, an alternative THINC-based interface sharpening approach is investigated and extended for use with the present model in Chapter 3. Several validation and benchmark cases demonstrate the robustness of the approach, including the secondary breakup of a droplet after its interaction with a shockwave and two and three-dimensional simulations of a liquid jet injected into a $M = 2$ crossflow. Chapter 4 presents a paper to be submitted to a physics based journal such as Physical Review Fluids. It includes a parametric study of the effects of surface tension and incident shock Mach number on the
breakup process of a liquid column. The simulations include the effects of surface tension, compressibility, and molecular diffusion. A variety of breakup modes are observed and correlate well to experimental observations while the impacts of surface tension on the drag coefficient and trajectory of the deforming columns are examined. Finally, conclusions are presented in Chapter 5.
CHAPTER 2. A FINITE-VOLUME HLLC-BASED SCHEME FOR
COMPRESSIBLE INTERFACIAL FLOWS WITH SURFACE TENSION

A paper submitted to the Journal of Computational Physics

Daniel P. Garrick\textsuperscript{1}, Mark Owkes\textsuperscript{2}, \& Jonathan D. Regele\textsuperscript{3}

Abstract

Shock waves are often used in experiments to create a shear flow across liquid droplets to study secondary atomization. Similar behavior occurs inside of supersonic combustors (scramjets) under startup conditions, but it is challenging to study these conditions experimentally. In order to investigate this phenomenon further, a numerical approach is developed to simulate compressible multiphase flows under the effects of surface tension forces. The flow field is solved via the compressible multicomponent Euler equations (i.e., the five equation model) discretized with the finite volume method on a uniform Cartesian grid. The solver utilizes a total variation diminishing (TVD) third-order Runge-Kutta method for time-marching and second order TVD spatial reconstruction. Surface tension is incorporated using the Continuum Surface Force (CSF) model. Fluxes are upwinded with a modified Harten-Lax-van Leer Contact (HLLC) approximate Riemann solver. An interface compression scheme is employed to counter numerical diffusion of the interface. Both the HLLC solver and interface compression scheme are extended to account for capillary force terms and the associated pressure jump. A simple method for numerically computing the interface curvature is developed and an acoustic scaling of the surface tension coefficient is proposed for the non-dimensionalization of the model. The

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model captures the surface tension induced pressure jump exactly if the exact curvature is known and is further verified with an oscillating elliptical droplet and a Mach 3 shock droplet interaction problem.

2.1 Introduction

The current research is motivated by the importance of fuel atomization in high-speed propulsion systems. Efficient combustion is greatly dictated by the fuel-injection geometry but there is a limited understanding of the effect of design parameters on the atomization process [3], consisting of primary and secondary atomization. Primary atomization is represented by the initial breakup of a liquid sheet or jet into smaller drops or filaments. Droplets formed during primary atomization can further deform and breakup during secondary atomization. Numerical modeling can supplement experimental insights in understanding the physical processes involved during atomization, especially in flow regimes or at length scales which are otherwise difficult or impossible to measure experimentally. As of yet, little numerical work has been performed on the effects of surface tension on the atomization process in a supersonic compressible crossflow.

The secondary atomization process has been studied in some detail both experimentally and numerically (see [6] for a thorough review) and is characterized primarily by the Weber number which relates the surface tension and inertial forces. Spurred largely by the development of the Continuum Surface Force (CSF) method [22] which incorporates surface tension into the fluid governing equations as a volume force, surface tension has been studied numerically in a wide variety of incompressible applications, e.g. [18, 19, 20]. However, numerical simulations of atomization in the high Mach number regime thus far have focused on the early stages of droplet breakup where surface tension effects are not expected to play a significant role and are neglected [15, 16].

The multiphase nature of the flow requires an adequate description of the interface between the gas and liquid. As most applications of primary atomization occur at low Mach numbers [17], numerical modeling has largely focused on the incompressible regime where interface tracking methods [42, 44] have become popular. Many different interface tracking methods
exist and generally involve some type of deforming mesh or particle tracking for the purposes of reconstructing the interface. Such methods guarantee a sharp interface which allows for natural modeling of immiscible fluids and interfacial physics. While many of these methods have been extended to compressible formulations [36, 46, 47, 50] they are generally geometrically complex and can be difficult to implement in multiple spatial dimensions.

An alternative approach is the interface capturing method [55, 56, 57, 69] which generally involves advecting a volume fraction or level set function. Analogous to shock capturing schemes developed to handle flow discontinuities in compressible flow algorithms, it can easily handle large topology changes in the interface. The method adds an additional conservation equation and is simple to implement in multiple dimensions but often requires numerical smearing of the material interface. In the presence of large density ratios and strong shocks this smearing can generate significant errors in computations of shock-interface interactions [27]. One option to counter numerical diffusion of the interface is implementation of high resolution WENO reconstruction [59, 60]. While the method can accurately capture material interfaces and has been successfully used to simulate the early stages of droplet breakup [16], the non-TVD nature of the WENO scheme may cause difficulties in computation of interface curvature, a required parameter for incorporating surface tension. Another option is to employ TVD spatial reconstruction with flux limiting and an interface compression technique shown to be successful in countering the numerical smearing of the interface. Such an approach was shown to accurately compute shock-interface interaction in the presence of high density ratios and strong shocks despite being discretely non-conservative [58]. The interface compression scheme has since been further developed with non-linear preconditioning [27] and incorporated into physical timestepping with consistent thermodynamics [63]. However, the surface tension induced pressure jump across the interface has not yet been accounted for in the interface compression scheme.

For compressible multicomponent flows, it is common to assume pressure and velocity equilibrium among the fluid components. This results in a five equation model with separate mass conservation equations for each phase, a quasi-conservative advection equation for the volume fraction, and a single momentum and energy equation for the total mixture. This assumption has been successfully applied to previous compressible models with capillary forces featuring
all-speed relaxation [25] and exact [23] Riemann solvers that account for surface tension effects. Examples utilizing the HLLC Riemann solver include Le Martelot et al. [70] who developed a low speed model with surface tension for simulating nucleating boiling flows and Shukla [27] who demonstrated results with surface tension. Recently, a compressible framework utilizing the non-equilibrium seven equation Baer-Nunziato model [28] was developed with surface tension effects incorporated into a path-conservative Osher-type Riemann solver. However, specifically accounting for the surface tension induced pressure jump within the HLLC approximate Riemann solver remains to be discussed.

The objective of this work is to develop an efficient finite volume method for simulating high speed compressible flows with surface tension effects. Specifically, this includes developments to account for the surface tension induced pressure jump within the HLLC Riemann solver and the interface compression algorithm. Also, a simple and efficient method for computing interface curvature is developed and an acoustic non-dimensional scaling for the surface tension forces is proposed. For brevity, viscous forces are ignored and their inclusion will be the subject of future work.

The paper is organized as follows. Section 2.2 describes the model details including the governing equations, mixture rules, interface compression scheme, curvature computation, and the non-dimensionalization. Section 2.3 describes the spatial and temporal discretization of the overall method including the surface tension source terms and the interface compression scheme. Section 2.4 describes the one and two dimensional test cases used to verify the approach including simulations with both exact and numerically computed curvature values, comparisons with analytical solutions, and application of the method to a shock droplet interaction problem. This is followed with conclusions in Section 2.5.

### 2.2 Governing equations

The five equation model of Allaire [57] is employed in conjunction with capillary force terms written in a non-conservative form. As such, the compressible multicomponent Euler equations
govern the flowfield [23]:

\[
\frac{\partial \rho_l \phi_l}{\partial t} + \nabla \cdot (\rho_l \phi_l \mathbf{u}) = 0, \tag{2.1a}
\]

\[
\frac{\partial \rho_g \phi_g}{\partial t} + \nabla \cdot (\rho_g \phi_g \mathbf{u}) = 0, \tag{2.1b}
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) = \sigma \kappa \nabla \phi_l, \tag{2.1c}
\]

\[
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{u}) = \sigma \kappa \nabla \phi_l \cdot \mathbf{u}, \tag{2.1d}
\]

\[
\frac{\partial \phi_l}{\partial t} + \mathbf{u} \cdot \nabla \phi_l = 0, \tag{2.1e}
\]

where \(\rho_l \phi_l\), \(\rho_g \phi_g\), and \(\rho\) are the liquid, gas, and total densities, \(\mathbf{u} = (u, v)^T\) is the velocity, \(\phi_l\) is the liquid volume fraction, \(p\) is the pressure, \(\sigma\) is the surface tension coefficient, \(\kappa\) is the interface curvature, and \(E\) is the total energy

\[
E = \rho e + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u} \tag{2.2}
\]

where \(e\) is the specific internal energy. The fluid components are considered immiscible and the liquid and gas volume fraction functions (\(\phi_l\) and \(\phi_g\)) are used to capture the fluid interface. Mass is discretely conserved for each phase via individual mass conservation equations. Surface tension is implemented as a volume force as in the CSF model [22] with terms in both the momentum and energy equations [23]. While a conservative form of the surface tension force exists [71], the present model utilizes the non-conservative form which enables flexible treatment of the curvature term \(\kappa\) and its accuracy. Prior compressible flow models have employed both the conservative [23, 27] and non-conservative [25, 28, 70] model for surface tension.

### 2.2.1 Mixture rules

The diffuse interface capturing approach results in the material interface being spread over several grid cells. In this diffuse region, the fluid is treated as a mixture that is neither purely gas nor liquid. Flow variables within this mixture region are defined as follows. The gas (\(g\)) and liquid (\(l\)) volume fractions are related by

\[
\phi_g = 1 - \phi_l. \tag{2.3}
\]
The total density is given by
\[ \rho = \rho_l \phi_l + \rho_g \phi_g \]  
(2.4)

with internal energy
\[ \rho e = \rho_l \phi_l e_l + \rho_g \phi_g e_g. \]  
(2.5)

Utilizing an isobaric assumption [57, 60] and the stiffened gas equation of state (EOS) [72]
\[ p = (\gamma - 1)\rho e - \gamma \pi_{\infty} \]  
(2.6)

the EOS parameters are given by
\[ \Gamma = \frac{1}{\gamma - 1} = \frac{\phi_g}{\gamma - 1} + \frac{\phi_l}{\gamma_l - 1}, \]  
(2.7)
\[ \Pi = \frac{\gamma \pi_{\infty}}{\gamma - 1} = \frac{\phi_g \gamma_{\infty} \pi_{\infty, g}}{\gamma_g - 1} + \frac{\phi_l \gamma_{\infty} \pi_{\infty, l}}{\gamma_l - 1}, \]  
(2.8)

such that the total energy can be written as
\[ E = \Gamma p + \Pi + \frac{1}{2} \rho u \cdot u. \]  
(2.9)

The isobaric assumption has been successfully employed in prior work to simulate surface tension in a compressible multicomponent framework [23, 25, 27, 70]. Finally, the mixture speed of sound is given by
\[ c = \sqrt{\frac{\gamma (p + \pi_{\infty})}{\rho}} \]  
(2.10)

where the mixture quantities \( \gamma \) and \( \pi_{\infty} \) are computed using Eqs. 2.7 and 2.8. The mixture rules described above only apply in the diffuse interface region and simplify to either the gas or liquid parameters elsewhere.

### 2.2.2 Surface tension induced pressure jump

The eigensystem associated with Eqs. 2.1a-2.1e is outlined in Appendix A. The eigenvalues are identical to the standard Euler system however surface tension terms appear in the eigenvectors. These terms result in a surface tension induced pressure jump across the contact wave (\( \ast \)) given by (see [23])
\[ \Delta p_{\ast} = \sigma \kappa \Delta \phi_l. \]  
(2.11)
Figure 2.1 A liquid droplet in gas under ambient conditions experiences a pressure jump $\Delta p$ based on the surface tension coefficient $\sigma$ and droplet curvature $\kappa$. For the two-dimensional case the curvature of a circular droplet is $1/R$ where $R$ is the droplet radius.

This jump is consistent with the surface tension induced pressure jump described by the Young-Laplace law, i.e. see Figure 2.1:

$$\Delta p = \sigma \kappa. \quad (2.12)$$

From Eq. 2.11, any jump in liquid volume fraction $\phi_l$ is associated with a corresponding pressure jump as a function of the curvature and surface tension coefficient. If the material interface is sharpened with an interface compression scheme, the liquid volume fraction distribution is modified near the interface and the corresponding pressure jump should also be modified according to Eq. 2.11 to ensure the interface remains in equilibrium.

2.2.3 Interface compression

Material interfaces become smeared over time due to numerical diffusion. This can cause significant errors in the solution especially in the presence of shocks and rarefaction waves [27, 58]. To counter this numerical smearing an interface compression technique is employed. The method numerically maintains the gas-liquid immiscibility condition by sharpening the material interface to only a few grid cells throughout the simulation. A form of the interface compression technique developed by Shukla et al. [58] with thermodynamically compatible extensions developed by Tiwari et al. [63] is employed in the present research with additional modifications to account for surface tension effects. With the method, a compression step in pseudo-time $\tau$ is performed after each physical timestep. Compression is performed by solving
\[ \frac{\partial \rho_l \phi_l}{\partial \tau} = \hat{\mathcal{R}}_l, \quad (2.13a) \]
\[ \frac{\partial \rho_g \phi_g}{\partial \tau} = \hat{\mathcal{R}}_g, \quad (2.13b) \]
\[ \frac{\partial \rho u}{\partial \tau} = u \hat{\mathcal{R}}, \quad (2.13c) \]
\[ \frac{\partial E}{\partial \tau} = \kappa_e \hat{\mathcal{R}} + \left[ p(\Gamma_l - \Gamma_g) + \Pi_l - \Pi_g \right] \mathcal{R} \]
\[ + \sigma \kappa (\gamma_l \phi_g + \gamma_g \phi_l + (\gamma_g - \gamma_l) \Delta \tau \mathcal{R} - 1) \Gamma_l \Gamma_g \mathcal{R}, \quad (2.13d) \]
\[ \frac{\partial \phi_l}{\partial \tau} = \mathcal{R} \quad (2.13e) \]

over the computational pseudo-timestep \( \Delta \tau \) where \( \kappa_e = u \cdot u \) and \( \hat{\mathcal{R}} = \hat{\mathcal{R}}_l + \hat{\mathcal{R}}_g \). The compression operators \( \mathcal{R}, \hat{\mathcal{R}}_l, \) and \( \hat{\mathcal{R}}_g \) are defined as:

\[ \mathcal{R} = n \cdot \left[ \nabla (\epsilon_h |\nabla \phi_l|) - \phi_l (1 - \phi_l) \right], \quad (2.14) \]
\[ \hat{\mathcal{R}}_l = H n \cdot \left[ \nabla (\epsilon_h n \cdot \nabla (\rho_l \phi_l)) - (1 - 2\phi_l) \nabla (\rho_l \phi_l) \right], \quad (2.15) \]
\[ \hat{\mathcal{R}}_g = H n \cdot \left[ \nabla (\epsilon_h n \cdot \nabla (\rho_g \phi_g)) - (1 - 2\phi_l) \nabla (\rho_g \phi_g) \right] \quad (2.16) \]

where the interface thickness is determined by the dissipation parameter \( \epsilon_h \) which is set by the user. Following [27], \( \epsilon_h = 0.5h \) and \( 0.72h \) are employed for one and two dimensional simulations, respectively. Density variations can occur outside the interface region due to the compressible nature of the flow. The Heaviside function \( H \) restricts the density compression to the interface region using [58]:

\[ H = \tanh \left( \frac{\phi_l (1 - \phi_l)}{10^{-2}} \right)^2 \]. \quad (2.17) \]

The second-order accurate centered finite volume spatial discretization described by Shukla et al. in [58] is employed for the compression scheme and is outlined in Section 2.3.3 for completeness. See the work of Tiwari et al. [63] for discussion of consistent compression of all conservative variables.

The \( \sigma \kappa \) term in the energy compression equation (Eq. 2.13d) accounts for the surface tension effects. From Eq. 2.38, the pressure jump due to the surface tension coincides with the jump in volume fraction \( \phi_l \) across the interface. To remain consistent, as the interface compression sharpens \( \phi_l \), the surface tension pressure jump must also be sharpened. This is
further complicated by the compression being applied to the energy directly - specifically the pressure contribution to energy $\Gamma p$. In the current model, both $\Gamma$ (via the mixture rules if $\gamma_g \neq \gamma_l$) and $p$ (via surface tension) are functions of $\phi_l$ in the diffused mixture region. The interaction between these terms in the energy (from $\Gamma p$) contributes the non-linear portion (i.e. $R^2$) of the surface tension compression term in Eq. 2.13d.

The surface tension sharpening term can be derived by considering a compression step performed on the interface of a static droplet. This is represented by a uniform pressure field with a surface tension induced pressure jump across the interface as a function of the curvature $\kappa$, surface tension coefficient $\sigma$, and liquid volume fraction $\phi_l$. Based on the conditions described above, the exact energy distribution at an initial pseudo-time $\tau$ can be represented by:

$$E^\tau = \Gamma^\tau (p + \sigma\kappa\phi_l^\tau) + \Pi^\tau$$  \hspace{1cm} (2.18)

where $\Gamma^\tau = \phi_l^\tau \Gamma_l + (1 - \phi_l^\tau) \Gamma_g$ and $\Pi^\tau = \phi_l^\tau \Pi_l + (1 - \phi_l^\tau) \Pi_g$. After marching forward in pseudo time with a compression timestep $\Delta \tau$, the resulting volume fraction and energy distributions should again satisfy the exact pressure jump across the interface

$$\phi_l^{\tau+\Delta \tau} = \phi_l^\tau + \Delta \tau \mathcal{R},$$  \hspace{1cm} (2.19)

$$E^{\tau+\Delta \tau} = \Gamma^{\tau+\Delta \tau} (p + \sigma\kappa\phi_l^{\tau+\Delta \tau}) + \Pi^{\tau+\Delta \tau}$$  \hspace{1cm} (2.20)

where $\Gamma^{\tau+\Delta \tau}$ and $\Pi^{\tau+\Delta \tau}$ are calculated using $\phi_l^{\tau+\Delta \tau}$ from Eq. 2.19 and the mixture rules given by Eqs. 2.7 and 2.8.

It can be shown that this compression scheme maintains equilibrium in the interface in the case where, for simplicity, $\gamma_g = \gamma_l = \gamma$ and $\pi_{\infty,g} = \pi_{\infty,l} = 0$ such that $\Gamma_l = \Gamma_g = \Gamma$, $\Gamma^{\tau+\Delta \tau} = \Gamma^{\tau}$, and $\Pi = 0$. Substituting these into Eq. 2.13d and advancing in pseudo-time by $\Delta \tau$ leads to:

$$E^{\tau+\Delta \tau} = E^\tau + \Delta \tau \sigma \kappa \Gamma \mathcal{R}$$  \hspace{1cm} (2.21)

$$E^{\tau+\Delta \tau} = \Gamma (p + \sigma \kappa \phi_l^{\tau+\Delta \tau}) + \Delta \tau \sigma \kappa \Gamma \mathcal{R}.$$  \hspace{1cm} (2.22)

To remain consistent, the pressure jump should coincide with the newly compressed volume fraction so the energy distribution should correspond to:

$$E^{\tau+\Delta \tau} = \Gamma (p + \sigma \kappa \phi_l^{\tau+\Delta \tau}).$$  \hspace{1cm} (2.23)
which on substituting Eq. 2.19 for $\phi_l^{\tau+\Delta \tau}$ gives

$$E^{\tau+\Delta \tau} = \Gamma(p + \sigma \kappa \phi_l^\tau) + \Delta \tau \sigma \kappa \Gamma R.$$ (2.24)

Clearly Eqs. 2.22 and 2.24 are equivalent meaning the pressure jump due to surface tension is sharpened in a manner consistent with the associated volume fraction and the equilibrium in the interface is maintained. This will also be demonstrated numerically in Section 2.4.2 for the more general case where $\gamma_g \neq \gamma_l$ and $\pi_{\infty,g} \neq \pi_{\infty,l}$.

The interface compression scheme works in concert with the diffuse interface approach such that the interface remains sharp but with a mesh-representable profile. This allows gradients across the discontinuous interface to be calculated with reasonable accuracy. For example, to perform interface compression, the interface normals must first be computed. This procedure and the interface curvature calculation is discussed in the following section.

### 2.2.4 Curvature computation

Interface curvature is calculated via the interface normals

$$\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \left( \frac{\nabla \psi}{|\nabla \psi|} \right)$$ (2.25)

where $\psi$ is a smoothed interface function [58]

$$\psi = \frac{\phi_l^\alpha}{\phi_l^\alpha + (1 - \phi_l)^\alpha}$$ (2.26)

where $\alpha = 0.1$. The vector quantity $\nabla \psi$ (and thus the normals) is calculated using fourth order central differences while the curvature itself, i.e.,

$$\kappa = -\nabla \cdot \mathbf{n}$$ (2.27)

is calculated using a second order central difference. This approach is found to improve convergence of the curvature calculation compared to utilizing second order differences for both the normal and curvature calculation.

The present work also incorporates an interfacial (as opposed to spatial) filtering strategy to locally improve the quality of the curvature calculation in the vicinity of the interface. The
$n + 1$ value of curvature at cell $i, j$ is corrected using weighted curvature values at iteration $n$ by:

$$
\kappa_{i,j}^{n+1} = \frac{\sum_{k=1}^{9} w_k \kappa_k^n}{\sum_{k=1}^{9} w_k}
$$

(2.28)

where $k$ refers to the $(i, j)$ index in the nine point stencil immediately surrounding the point $i, j$, i.e. $(i, j), (i + 1, j), (i + 1, j + 1)$, etc. The weighting factor is

$$
w_k = (\phi_l(1 - \phi_l))^2_k
$$

(2.29)

which weights the local curvature to the value at the center of the interface at $\phi_l = 0.5$. The curvature is calculated and corrected at the end of each physical timestep before interface compression is performed. Figure 2.2(a) depicts the effect the filtering strategy has on correcting the curvature distribution near the interface. For a droplet centered at $(0, 0)$ the numerically computed curvature follows $1/r$ where $r = \sqrt{x^2 + y^2}$ is the local cell center value. The exact curvature for a two dimensional circular droplet is a constant $1/R$ where $R$ is the radius of the droplet. The filtering strategy drives the curvature distribution within the interface to the local value at $\phi_l = 0.5$ which corresponds to the actual interface location if it were infinitely thin.

A grid convergence study is performed for the curvature calculation. The $L_2$ error defined by

$$
L_2 = \sqrt{\frac{1}{N} \sum (\kappa_{i,j} - \frac{1}{R})^2}
$$

(2.30)

is computed where $\frac{1}{R}$ is the exact curvature and $\kappa_{i,j}$ is the numerically computed curvature in cell $i, j$. As the surface tension force (and curvature) is only applied in the diffuse interface region, $N$ is taken as the number of grid points within this region defined by the computational cells where $\phi_l(1 - \phi_l) > 0.001$. The results are depicted in Figure 2.2(b) and indicate that second order accuracy is obtained when ten correction iterations are applied. Five iterations shows a significant reduction in the error compared to the directly computed curvature but exhibits first order convergence. The effect of the correction iterations in practice can be seen in Section 2.4.3.
(a) Effect of correction iterations on curvature distribution. In essence, the curvature value is locally driven to its value at the center of the interface, corresponding to the curvature value of an infinitely thin interface. The theoretical first and second order convergence are given by the solid lines. No correction refers to the curvature calculated directly from Eq. 2.25.

Figure 2.2 Convergence of curvature distribution.

2.2.5 Final model and non-dimensionalization

With the various ingredients of the overall model now specified, the non-dimensionalization of the governing equations follows. Substituting dimensional quantities using the non-dimensional rules in Table 2.1 into Eqs. 2.1a-2.1e results in the final non-dimensional model:

\[
\frac{\partial \rho_l \phi_l}{\partial t} + \nabla \cdot (\rho_l \phi_l u) = 0, \\
\frac{\partial \rho_g \phi_g}{\partial t} + \nabla \cdot (\rho_g \phi_g u) = 0, \\
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u + p \tilde{I}) = \frac{1}{W_e a} \kappa \nabla \phi_l, \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p) u) = \frac{1}{W_e a} \kappa \nabla \phi_l \cdot u, \\
\frac{\partial \phi_l}{\partial t} + u \cdot \nabla \phi_l = 0,
\]

in conjunction with the stiffened gas EOS written in terms of the mixture rules (Eqs. 2.7-2.8):

\[
E = \Gamma p + \Pi + \frac{1}{2} \rho u \cdot u.
\]
Table 2.1 Non-dimensional rules used in the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>( x = x'/l' )</td>
</tr>
<tr>
<td>Time</td>
<td>( t = t'a'_0/l' )</td>
</tr>
<tr>
<td>Velocity</td>
<td>( u = u'/a'_0 )</td>
</tr>
<tr>
<td>Density</td>
<td>( \rho = \rho'/\rho'_0 )</td>
</tr>
<tr>
<td>Pressure</td>
<td>( p = p'/\rho'_0a'_0^2 )</td>
</tr>
<tr>
<td>Total Energy</td>
<td>( E = E'/\rho'_0a'_0^2 )</td>
</tr>
<tr>
<td>Curvature</td>
<td>( \kappa = \kappa'l' )</td>
</tr>
<tr>
<td>Surface tension coefficient</td>
<td>( \sigma = \frac{1}{We_a} = \frac{\sigma'}{\rho'_0a'_0^2} )</td>
</tr>
</tbody>
</table>

This non-dimensionalization results in the surface tension force being scaled by an acoustic Weber number defined as:

\[
We_a = \frac{\rho'_0a'_0^2l'}{\sigma'}
\]

(2.32)

where \( \sigma' \) is the dimensional surface tension coefficient. For a static droplet of diameter \( l' \) in a moving freestream defined by \( u'_0 \) and \( \rho'_0 \) the physical Weber number can be determined as

\[
We = \frac{\rho'_0u'_0^2l'}{\sigma'} = We_aM^2
\]

(2.33)

where the Mach number is \( M = u'_0/a'_0 \).

### 2.3 Numerical method

The final model (Eqs. 2.31a-2.31e) is discretized using the finite volume method on a uniform \((\Delta x = \Delta y = h)\) Cartesian grid. The resulting semi-discrete form of the equations is given by:

\[
\frac{dQ_{i,j}}{dt} = -\left(\frac{f_{i+1/2} - f_{i-1/2}}{\Delta x}\right) - \left(\frac{g_{j+1/2} - g_{j-1/2}}{\Delta y}\right) + S_{i,j} + R(Q_{i,j})
\]

(2.34)

where \( Q \) is the vector of state variables, \( f \) and \( g \) are the conservative convective fluxes in the \( x \) and \( y \) directions, \( S_{i,j} \) is the source term, and \( R(Q_{i,j}) \) is the residual function. Spatial reconstruction is performed on the primitive variables using a TVD second order accurate scheme with the minmod limiter.
The conserved variables are then integrated in time using the following third order TVD Runge-Kutta scheme [73]:

\[
\begin{align*}
Q^{(1)}_{i,j} &= Q^n_{i,j} + \Delta t R(Q^n_{i,j}), \\
Q^{(2)}_{i,j} &= \frac{3}{4}Q^n_{i,j} + \frac{1}{4}Q^{(1)}_{i,j} + \frac{1}{4}\Delta t R(Q^{(1)}_{i,j}), \\
Q^{n+1}_{i,j} &= \frac{1}{3}Q^n_{i,j} + \frac{2}{3}Q^{(2)}_{i,j} + \frac{2}{3}\Delta t R(Q^{(2)}_{i,j}).
\end{align*}
\]

(2.36)

### 2.3.1 HLLC numerical flux and surface tension modifications

The fluxes are upwinded using the HLLC approximate Riemann solver [74, 75]. To ensure oscillation free advection of material interfaces, the primitive variables are reconstructed and the HLLC features adaptations for a quasi-conservative form of the volume fraction transport equation [59]. The present work includes several straightforward modifications to the HLLC solver to account for surface tension effects. The HLLC solver restores the contact wave by considering two separate states in the star region (see Figure 2.3) such that the HLLC flux \( \hat{f} \) is defined by

\[
\hat{f} = \begin{cases} 
  f_L & \text{if } 0 \leq s_L \\
  f_{*L} & \text{if } s_L \leq 0 \leq s_* \\
  f_{*R} & \text{if } s_* \leq 0 \leq s_R \\
  f_R & \text{if } 0 \geq s_R.
\end{cases}
\]

(2.37)

The standard HLLC solver [74] without surface tension assumes a single pressure value \( p_* \) across the contact discontinuity, i.e. \( p_* = p_{*L} = p_{*R} \). The left and right states in the star region should be modified such that the pressure jump imposed by Eq. 2.11 is captured. Eq. 2.11 is written in terms of the right \( R \) and left \( L \) states of the Riemann problem as

\[
p_{*R} - p_{*L} = \sigma \kappa (\phi_{l,R} - \phi_{l,L}).
\]

(2.38)

The present work accounts for this pressure jump by defining \( p_* \) as:

\[
p_* = p'_{*L} = p'_{*R}
\]

(2.39)

where the primed left and right star region pressures are given by

\[
p'_{*L} = p_{*L} - \sigma \kappa \phi_{l,L}, \quad p'_{*R} = p_{*R} - \sigma \kappa \phi_{l,R}
\]

(2.40)
Figure 2.3 The Riemann fan for the HLLC Riemann solver considers two different states within the middle (*) region separated by a middle wave speed \( s_* \), the contact wave. The left and right wave speeds are given by \( s_L \) and \( s_R \) respectively. The conserved variables in each region are denoted by \( Q_L, Q_R, Q_*L, \) and \( Q_*R \).

where \( p_{*L} \) and \( p_{*R} \) are defined as usual in HLLC:

\[
p_{*L} = p_L + \rho_L(s_L - u_L)(s_* - u_L), \quad p_{*R} = p_R + \rho_R(s_R - u_R)(s_* - u_R).
\]

(2.41)

Using Eq. 2.39, the middle wave speed \( s_* \) is now determined to be

\[
s_* = \frac{p_R - p_L + \rho_L u_L(s_L - u_L) - \rho_R u_R(s_R - u_R) - \sigma \kappa (\phi_{L,R} - \phi_{l,L})}{\rho_L(s_L - u_L) - \rho_R(s_R - u_R)}.
\]

(2.42)

The final form of the HLLC flux is given compactly by [60]

\[
\hat{f} = \frac{1 + \text{sgn}(s_*)}{2} \left[ f_L + s_-(Q_*L - Q_L) \right] + \frac{1 - \text{sgn}(s_*)}{2} \left[ f_R + s_+(Q_*R - Q_R) \right]
\]

(2.43)

in conjunction with the numerical flux \( f \) (\( g \) for the \( y \) direction) and state vector \( Q \) given by

\[
Q = \begin{pmatrix}
\rho \phi_l \\
\rho_g \phi_g \\
\rho u \\
\rho v \\
E \\
\phi_l
\end{pmatrix}, \quad f = \begin{pmatrix}
\rho \phi_l u \\
\rho_g \phi_g u \\
\rho u + p \\
\rho v \\
(E + p)u \\
\phi_l u
\end{pmatrix}, \quad g = \begin{pmatrix}
\rho \phi_l v \\
\rho_g \phi_g v \\
\rho v + p \\
\rho v + p \\
(E + p)v \\
\phi_l v
\end{pmatrix},
\]

(2.44)
where the intermediate state is (for the $x$ direction)

$$
Q_{i,K} = \frac{s_K - u_K}{s_K - s^*} \begin{pmatrix}
(\rho_l \phi_l)_K \\
(\rho_g \phi_g)_K \\
\rho_K s^* \\
\rho_K v_K \\
E_K + (s^* - u_K) \left(\rho_K s^* + \frac{p_K - \sigma \phi_l}{s_K - u_K}\right) \\
\phi_l
\end{pmatrix}
$$

(2.45)

where $K = L, R$ refers to the left and right cell states and the curvature is defined here as $

\kappa = \frac{1}{2}(\kappa_L + \kappa_R)$ where $\kappa_L$ and $\kappa_R$ are the curvatures defined at the cell center of the left and right cells, respectively. The wave speeds are computed using [76]

$$
s_- = \min(0, s_L), \quad s_+ = \max(0, s_R)
$$

(2.46)

where

$$
s_L = \min(\bar{u} - \bar{c}, u_L - c_L), \quad s_R = \max(\bar{u} + \bar{c}, u_L + c_L)
$$

(2.47)

where, following [60], $\bar{u} = \frac{1}{2}(u_L + u_R)$ and $\bar{c} = \frac{1}{2}(c_L + c_R)$. Note that far from the interface ($\phi_{i,R} - \phi_{i,L} = 0$) or in the case of no surface tension ($\sigma = 0$) this choice of wave speeds is identical to that of Batten et al. [77] but now accounts for surface tension effects near the interface. Note that the HLLC is applied on a direction by direction basis and is straightforward to extend to multiple dimensions.

Following Johnsen and Colonius [59] the advection equation is written in quasi-conservative form

$$
\frac{\partial \phi_l}{\partial t} + \nabla \cdot (\phi_l \mathbf{u}) = \phi_l \nabla \cdot \mathbf{u}
$$

(2.48)

where the source term is evaluated within the $i, j$ computational cell using

$$
(\phi_l \nabla \cdot \mathbf{u})_{i,j} = (\phi_l)_{i,j} \left[ \frac{1}{\Delta x} (u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}) + \frac{1}{\Delta y} (v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}) \right]
$$

(2.49)

where the velocity at the face is determined from the HLLC solver by

$$
u_{i-\frac{1}{2},j} = \hat{u}(Q_{i-\frac{1}{2},j}^L, Q_{i-\frac{1}{2},j}^R)
$$

(2.50)
where

\[
\hat{u} = \frac{1 + sgn(s_*)}{2} \left[ u_L + s_\left( \frac{s_L - u_L}{s_L - s_*} - 1 \right) \right] + \frac{1 - sgn(s_*)}{2} \left[ u_R + s_\left( \frac{s_R - u_R}{s_R - s_*} - 1 \right) \right].
\]  

(2.51)

### 2.3.2 HLLC surface tension source terms

The present work includes additional modifications of the HLLC solver to account for the surface tension source terms. For the surface tension force in the \( u \) momentum equation:

\[
\sigma \kappa \frac{\partial \phi}{\partial x} = \sigma \kappa_{i,j} \left[ \frac{1}{\Delta x} (\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}) \right].
\]  

(2.52)

The force in the \( v \) momentum equation is treated similarly. For consistency, the velocity used in the source term should be the same as that used in the advective numerical flux [59, 60]. To achieve this, similarly to the advection equation, the surface tension source term in the energy equation is first decomposed into conservative and non-conservative terms using

\[
\nabla \cdot (\phi \mathbf{u}) = \phi \nabla \cdot \mathbf{u} + \nabla \phi \cdot \mathbf{u}
\]  

(2.53)

such that

\[
(\sigma \kappa \nabla \phi) \cdot \mathbf{u} = \sigma \kappa \left[ \nabla \cdot (\phi \mathbf{u}) - \phi \nabla \mathbf{u} \right]
\]  

(2.54)

\[
= \sigma \kappa_{i,j} \left[ \frac{1}{\Delta x} \left( (\phi u)_{i+\frac{1}{2},j} - (\phi u)_{i-\frac{1}{2},j} \right) + \frac{1}{\Delta y} \left( (\phi v)_{i,j+\frac{1}{2}} - (\phi v)_{i,j-\frac{1}{2}} \right) \right]
\]  

\[
- \phi_{i,j} \left( \frac{1}{\Delta x} \left( u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j} \right) + \frac{1}{\Delta y} \left( v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}} \right) \right)
\]  

(2.55)

with

\[
(\phi u)_{i+\frac{1}{2},j} = \phi_{i+\frac{1}{2},j} u_{i+\frac{1}{2},j}.
\]  

(2.56)

The face values are determined from the HLLC solver for the volume fraction by

\[
\phi = \frac{1 + sgn(s_*)}{2} \phi_L + \frac{1 - sgn(s_*)}{2} \phi_R,
\]  

(2.57)

and velocity by Eq. 2.51.
2.3.3 Compression discretization

The compression operators \( R \) and \( \hat{R}_s = \hat{R}_l, \hat{R}_g \) are discretized as in the work of Shukla et al. [58] for the \( i,j \) computational cell as follows:

\[
R = \left( \frac{f_{i+1/2,j} - f_{i-1/2,j}}{\Delta x} \right) n_{i,j}^x + \left( \frac{g_{i,j+1/2} - g_{i,j-1/2}}{\Delta y} \right) n_{i,j}^y, \quad (2.58)
\]

\[
\hat{R}_s = H(\phi_{i,j}) \left[ \left( \frac{f_{i+1/2,j}^* - f_{i-1/2,j}^*}{\Delta x} \right) n_{i,j}^x + \left( \frac{g_{i,j+1/2}^* - g_{i,j-1/2}^*}{\Delta y} \right) n_{i,j}^y \right. \\
- \left. (1 - 2\phi_{i,j}) \left( \frac{(\rho_\ast \phi_\ast)_{i+1,j} - (\rho_\ast \phi_\ast)_{i-1,j}}{2\Delta x} n_{i,j}^x + \frac{(\rho_\ast \phi_\ast)_{i,j+1} - (\rho_\ast \phi_\ast)_{i,j-1}}{2\Delta y} n_{i,j}^y \right) \right] \quad (2.59)
\]

where the subscript \( l \) is dropped from the liquid volume fraction \( \phi_l \) for convenience, \(* = l, g\) denotes either the liquid or gas phasic densities, respectively, and \( H(\phi_{i,j}) \) is the Heaviside function given by Eq. 2.17. The fluxes are given by

\[
f_{i-1/2,j} = \epsilon_h |\nabla \phi|_{i-1/2,j} - (\phi(1 - \phi))_{i-1/2,j} \quad (2.60)
\]

\[
f_{i-1/2,j}^* = \epsilon_h n_{i-1/2,j} \cdot \nabla (\rho_\ast \phi_\ast)_{i-1/2,j} \quad (2.61)
\]

where

\[
(\phi(1 - \phi))_{i-1/2,j} = \phi_{i-1/2,j} - \phi_{i-1/2,j} \cdot (1 - \phi_{i-1/2,j}), \quad (2.62)
\]

\[
\phi_{i-1/2,j} = \frac{\phi_{i,j} + \phi_{i-1,j}}{2}. \quad (2.63)
\]

The normal is computed by

\[
n_{i-1/2,j} = \frac{\nabla \psi_{i-1/2,j}}{|\nabla \psi|_{i-1/2,j}} \quad (2.64)
\]

where \( \psi \) is the smoothed interface function described in Eq. 2.26. The gradients of \( \psi \) at the face are computed as

\[
(\psi_x)_{i-1/2,j} = \frac{\psi_{i,j} - \psi_{i-1,j}}{\Delta x}, \quad (2.65)
\]

\[
(\psi_y)_{i-1/2,j} = \frac{\psi_{i,j+1} - \psi_{i,j} - \psi_{i,j+1} - \psi_{i-1,j+1}}{4\Delta y}, \quad (2.66)
\]

with gradients of \( (\rho_\ast \phi_\ast) \) at the face calculated similarly. Finally, the gradient of the smoothed \( \psi \) function is related to the volume fraction gradient by [58]:

\[
|\nabla \phi|_{i-1/2,j} = \frac{1}{\alpha} \left( \phi(1 - \phi)_{i-1/2,j}^{1-\alpha} (\phi_{i-1/2,j}^\alpha + (1 - \phi_{i-1/2,j})^\alpha)^2 |\nabla \psi|_{i-1/2,j}. \quad (2.67)
\]

The gradients and flux values for the other faces and directions are treated similarly.
2.3.3.1 Compression timestepping

In the present work, as in that of Shukla et al. [58], the compression algorithm is performed as an independent “post-processing” step after each physical timestep has completed. Note that the present method differs from that of [58] in two ways. First, compression is performed directly on the conservative variables based on the work of Tiwari et al. [63] rather than the primitive variables as in [58]. The present compression scheme also differs in that the surface tension induced pressure jump across the interface is accounted for during the compression step. This compression step consists of a set of iterations advancing Eqs. 2.13a-2.13e in pseudo-time $\tau$ using the computational timestep $\Delta \tau$ until a steady state is reached and the desired interface thickness is recovered. For example, the $\phi_l$ compression equation (Eq. 2.13e) is advanced in pseudo-time via

$$\phi_l^{\tau+\Delta \tau} = \phi_l^{\tau} + \Delta \tau R$$

with the other compression equations treated similarly.

Note that Tiwari et al. [63] incorporates the compression step into the physical timestepping by scaling the compression operator $R$ by a characteristic interface velocity:

$$U = 4 \left( \phi_l (1 - \phi_l) |u| \right)_{max}.$$  

(2.69)

This essentially assumes that if the interface is not moving then numerical diffusion is minimal and interface compression is not needed. An analogous compression timestep for the present approach would be $\Delta \tau = U \Delta t$ where $\Delta t$ is the physical timestep size employed. Shukla et al. [58] utilized a constant compression timestep of $\Delta \tau = 0.2h$ where $h$ is the uniform grid spacing. The current work utilizes a constant $\Delta \tau = 0.1h$ and performs between one and five compression iterations per physical timestep depending on the ratio of $U \Delta t$ to $0.1h$. This provides a good balance between computational effort, stability, and maintaining the desired interface thickness throughout the simulation.

2.4 Results and discussion

To verify the numerical model and implementation, one dimensional testing is performed first. This begins with a standard gas-liquid shock tube problem without surface tension. This
is followed with two dimensional simulations of a circular droplet with surface tension to verify
the ability of the model to capture correctly the surface tension induced pressure jump. Final
verification is performed with spurious current and oscillating elliptical droplet tests. The
method is then applied to a Mach 3 shock droplet interaction problem.

2.4.1 Gas-liquid Riemann problem

To verify the solution algorithm is correctly implemented without surface tension, a gas-
liquid Riemann problem previously used as a model for underwater explosions [55, 78] and
verification of a multicomponent flow model [59, 60] is simulated. The problem includes highly
compressed air and water at atmospheric pressure. The non-dimensional initial conditions are
given by [78]:

\[
(\rho_l \phi_l, \rho_g \phi_g, u, p) = \begin{cases} 
(0, 1.241(1 - \phi_l), 0, 2.753) & -1 < x < 0 \\
(0.991\phi_l, 0, 0, 3.059 \times 10^{-4}) & 0 \leq x \leq 1
\end{cases}
\]

(2.70)

with fluid properties \( \gamma_l = 5.5, \pi_{\infty,l} = 1.505, \gamma_g = 1.4, \pi_{\infty,g} = 0 \). Note the material interface is
initialized in a slightly diffused state with an exponential function:

\[
\phi_l = 1 - \left(1 + \exp \frac{x}{\epsilon_h}\right)^{-1}
\]

(2.71)

where \( \epsilon_h = 0.5h \), \( x \) is the cell center location and \( h = 0.0025 \) is the grid spacing with 800 grid
points. The results at a simulation time of \( t = 0.2 \) and a constant timestep of \( \Delta t = 2.5 \times 10^{-4} \)
are shown in Figure 2.4 and compare well to the exact solution. The interface compression
scheme successfully maintains the sharp material interface throughout the simulation.

2.4.2 Static droplet with exact curvature

The following simulation illustrates the ability of the present model to capture the surface
tension induced pressure jump exactly if exact curvature is prescribed and shows the effect
of the surface tension term in the energy compression equation. Without this term, spurious
oscillations are introduced into the solution even for a simple static droplet with exact prescribed
curvature. The initial conditions correspond to a unity radius liquid droplet in a gas with
Figure 2.4 Data (○) at $t = 0.2$ using 800 grid points compared to the exact solution (−).
density ratio 1000 and a unity acoustic Weber number such that the surface tension induced pressure jump across the interface is dictated by Eq. 2.11, or in terms of the \( \phi_l \) distribution,
\[
\Delta p = \frac{\kappa}{W_{\infty}} \phi_l = \phi_l:
\]
\[
(\rho_l \phi_l, \rho_g \phi_g, u, v, p) = (1000 \phi_l, (1 - \phi_l), 0, 0, 1 + \Delta p).
\]

Following Shukla [27], the equation of state properties are chosen for air \((\gamma_g = 1.4, \pi_{\infty,g} = 0)\) and a water-like substance \((\gamma_l = 4.4, \pi_{\infty,l} = 100)\) so as not to significantly restrict the maximum timestep that can be taken. To demonstrate the effect of compression, the interface is initialized in an overly diffused state with \(\Delta = 2\) via:
\[
\phi_l = \left(1 + \exp \frac{r - 1}{\Delta \epsilon_h}\right)^{-1}
\]

with \(r = \sqrt{x^2 + y^2}\) and \(\epsilon_h = 0.72h\). Extrapolation boundary conditions are employed on a mesh with 80 \(\times\) 80 grid points \((h = 0.05)\) for a \([-2, 2] \times [-2, 2]\) domain. The solution is computed using a CFL condition of 0.6 to a final time of \(t = 10\).

Plots of the results along a diagonal cut from \((x, y) = (-2, -2)\) to \((2, 2)\) are depicted in Figure 2.5. The surface tension compression term appears only in the energy compression equation and does not affect the behavior of the compression scheme on the volume fraction distribution, as shown in Figure 2.5(a). The pressure distributions with and without the surface tension compression term are shown in Figure 2.5(b). As the curvature is forced to the exact value, the pressure jump should correspond directly to the jump in volume fraction as dictated by Eq. 2.11.

Table 2.2 compares the \(L_{\infty}\) norm of the error in the pressure and velocity distributions for the simulations. Since the droplet is initially static, the velocity field should remain zero if the pressure and surface tension forces are in equilibrium throughout the simulation. The spurious pressure oscillations observed if surface tension is not accounted for in the interface compression scheme are found to generate disturbances in the velocity field. The pressure error is measured by subtracting the ambient pressure and the exact pressure jump (according to Eq. 2.11) from the computed pressure. The results indicate that if the exact curvature is provided, the present model maintains equilibrium across the interface and captures the surface tension induced pressure jump to within machine precision.
Figure 2.5  The volume fraction $\phi_l$ (a) and pressure (b) is plotted over a diagonal cut from $(x, y) = (-2, -2)$ to $(2, 2)$. Lines depict the diffused initial conditions (−) and results at the final time with (−−) and without (··) the surface tension term included in the energy compression equation.

Table 2.2  $L_\infty$ norms of the pressure and velocity error for the simulation with exact curvature with and without the surface tension term included in the energy compression equation.

<table>
<thead>
<tr>
<th>Error</th>
<th>Surface tension compression term</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Included</td>
</tr>
<tr>
<td>Pressure ($\max</td>
<td>p - (1 + \Delta p)</td>
</tr>
<tr>
<td>Velocity ($\max</td>
<td>u</td>
</tr>
</tbody>
</table>
2.4.3 Parasitic currents

Errors in the calculation of the interface curvature can increase the magnitude of unphysical “parasitic currents” inherent in surface tension simulations [23, 79, 80]. As the current work does not include physical diffusion (i.e. \( Re \to \infty \), but numerical diffusion exists in practice), the effect of the parasitic currents could potentially be detrimental and should be investigated.

A simple test is performed to check if the currents distort the material interface. The same initial conditions as the previous test case are employed but without the overly diffused interface initialization, i.e. \( \Delta = 1 \) in Eq. 2.73 which corresponds to the interface width enforced by the solution of the interface compression algorithm at steady state. The droplet should remain stationary and the interface should not become distorted due to the parasitic currents. The curvature is calculated numerically using the procedure in Section 2.2.4 with five and ten correction iterations. The solution is advanced to non-dimensional time \( t = 100 \) using a CFL of 0.6.

Typically the effect of the parasitic currents are reported in terms of the Laplace number \( La = \rho \sigma D/\mu^2 \) and the capillary number measured as \( Ca = |u|_{max} \mu/\sigma \) (for example see [35, 81]). Since the current work does not include physical diffusion terms, these parameters are undefined. Instead, the maximum velocity during the spurious current test is depicted in Figure 2.6 for several grid resolutions. When five correction iterations (Figure 2.6(a)) are employed the currents gradually increase over time. With ten iterations (Figure 2.6(b)), the currents oscillate with time but the mean value remains almost constant. In both cases the maximum velocity is shown to decrease with mesh refinement. In all cases the currents remain small (on the order of \( 10^{-4} - 10^{-5} \)) and no signs of interface distortion are observed in any of the performed simulations. As physical diffusion terms are presently neglected and should damp the spurious currents, this result is satisfactory.

2.4.4 Oscillating ellipse

An oscillating ellipse study is frequently performed to validate the accuracy of surface tension implementations [23, 27, 54, 82] and ensure the model is capable of predicting physical
solutions. The period of oscillation can be computed analytically \[83, 84\]. The result has been non-dimensionalized here and is written as:

\[
T = 2\pi \sqrt{\frac{\text{We}_a(1 + \epsilon)R^3}{6}}
\]

where \(T\) is the oscillation period in non-dimensional time, \(\text{We}_a\) is the acoustic Weber number, \(\epsilon = \rho_l/\rho_g\) is the density ratio and \(R\) is the equivalent circular radius. An ellipse defined by

\[
1 = \frac{x^2}{a^2} + \frac{y^2}{b^2}
\]

has an equivalent circular radius of \(R = \sqrt{ab}\) assuming mass is conserved. Several oscillating ellipse simulations using \(a = 5/4\) and \(b = 4/5\) were performed for density ratios of 100 and 1000. The domain and material properties are the same as in the parasitic currents test above. All simulations were performed with a CFL of 0.6 with five curvature correction iterations. The numerical oscillation period was measured using the variation in global kinetic energy \(\frac{1}{2} \int \rho |\mathbf{u}|^2 dxdy\) where a full period occurs every other trough. Figure 2.7 shows the behavior of the global kinetic energy over time for several grid resolutions. Overall, excellent agreement was found with the analytical result, as shown in Figure 2.8 for a 200 × 200 grid.
Figure 2.7  Global kinetic energy for an oscillating elliptical droplet on a $50 \times 50$ (--), $100 \times 100$ (---), and $200 \times 200$ (--) grid for an acoustic Weber number of 1 and density ratio $\epsilon = 1000$. 

Figure 2.8  Analytical results for density ratios of $\epsilon = 100$ (--) and $\epsilon = 1000$ (---) compared to the computed (○) ellipse oscillation period as a function of the acoustic Weber number.
2.4.5 Droplet shock interaction

A shockwave traveling in air at a Mach number $M_s = 3$ is simulated impacting a water column with unity radius. The initial conditions correspond to those in [85] but non-dimensionalized by the column radius $r = 1.75$ mm and with different EOS parameters for the water given by $\gamma_l = 4.4$ and $\pi_{\infty,l} = 6 \times 10^8$ Pa [58]. The domain is $[-5, 10] \times [-5, 5]$ and extrapolation boundary conditions are applied on all four boundaries. At the end of the simulation the upstream inlet conditions are verified to be unchanged from the initial conditions which are given in non-dimensional form by

$$\begin{cases} (\rho_l \phi_l, \rho_g \phi_g, u, v, p) = (0, 3.857, 2.629, 0, 10.333) & x \leq -2/1.75 \\ (1000 \phi_l, (1 - \phi_l), 0, 0, 1 + \Delta p) & \text{otherwise} \end{cases}$$

(2.76)

where $\gamma_l = 4.4$, $\pi_{\infty,l} = 6000$, $\gamma_g = 1.4$ and $\pi_{\infty,g} = 0$ and

$$\phi_l = \left(1 + \exp \frac{r - 1}{\epsilon_h}\right)^{-1}$$

(2.77)

with $r = \sqrt{x^2 + y^2}$ and $\epsilon_h = 0.72h$. The acoustic Weber number is set to $\text{We}_a = 1.446$ making the initial pressure jump distribution $\Delta p = \phi_l/1.446$ for the simulation with surface tension. Note that the initial conditions correspond to a supersonic flow ($M = 1.358$) which generates a leading bow shock and a variation in local flow conditions over the droplet. Considering a stream-line emanating upstream from the stagnation point of the droplet the jump conditions across the bow shock can be estimated using normal shock relations. This provides an estimated upper bound of $\text{We} = 47.7$ for the physical Weber number. The same CFL and curvature correction settings as the oscillating ellipse simulation are employed.

Figure 2.9 depicts a numerical Schlieren (exponentially spaced normalized density gradient) of the early stages of the Euler simulation characterized by the incident shockwave impacting the water column. This results in a transmitted shockwave inside the column and a reflected bow shock upstream. The effects of surface tension are not significant at this stage. The results agree well with the previous AUSM-based simulation by Chang and Liou [85]. This includes a slight but expected variation in the transmitted shockwave location in the water column at later times due to the difference in the EOS parameters employed.
Figure 2.9  Numerical schlieren of the early stages of droplet shock interaction on a 2400 × 1600 grid for non-dimensional times of 0.1807, 0.3614, 0.5421, 0.7228, 1.0842, and 1.4456. Based on the droplet dimensions in [85], these correspond to physical times of 1, 2, 3, 4, 6, and 8 μs.
The effects with vs. without surface tension are examined in Figure 2.10 in terms of the overall flow structure. In the simulation without surface tension, increased grid resolution leads to the development of interfacial instabilities which tend to grow over time. These features are especially noticeable on the top and bottom of the water column and appear to generate local recirculation regions observed at \( t = 12 \). Similar flow features are not observed in the case with surface tension where the interface remains significantly smoother throughout the simulation.

The location of the gas-liquid interface is measured as the \( \phi_l = 0.5 \) iso-line. The surface tension actively combats the deformation of the drop as evidenced in Figure 2.11. Figure 2.12 shows the interface location at three different grid resolutions for the cases without (Figure 2.12(a)) and with (Figure 2.12(b)) surface tension. With surface tension it is observed that there is very little variation in the interface location between the different grid resolutions. This is contrasted with the increased interface instabilities that develop in the simulation without surface tension with increasing grid resolution.

### 2.5 Conclusion

A finite volume method is developed to simulate compressible multicomponent flow with capillary forces. An extension of the HLLC Riemann solver and an interface compression scheme are developed to account for the pressure jump across an interface from surface tension. If the exact curvature is known, the method is shown to capture the surface tension induced pressure jump to within machine precision for a static droplet. Additionally, a simple method for calculating the interface curvature is developed. In the case of a circular droplet, the interface curvature is shown to be second order accurate with sufficient correction iterations. Parasitic currents are found not to adversely affect the interface despite physical diffusion terms being neglected at this time. The overall method is further verified through comparisons to the analytical relationship of an oscillating elliptical droplet and a droplet shock interaction problem in a supersonic crossflow. The results highlight the effect of surface tension in combating drop deformation. The method was developed and tested in two-dimensions, but the extension to three dimensions is straightforward.
Figure 2.10  Numerical schlieren of later stages of simulations without surface tension (a) vs. with surface tension (b) at non-dimensional times of 6, 8, 10, 12. Based on the droplet dimensions in [85], these correspond to physical times of 33.2, 44.2, 55.3, 66.4 µs.
Figure 2.11 Interface iso-line for $\phi_l = 0.5$ with (−−) and without (−) surface tension on the $2400 \times 1600$ grid at non-dimensional times of 6, 8, 10, and 12.

(a) Without surface tension
(b) With surface tension

Figure 2.12 Grid resolution study of the interface function without (a) and with (b) surface tension on grids of $600 \times 400$ (−), $1200 \times 800$ (−−), and $2400 \times 1600$ (−) at a non-dimensional time of 12.
2.6 Acknowledgments

This work is supported by Taitech, Inc. under sub-contract TS15-16-02-004 (primary contract FA8650-14-D-2316).

Appendix A: Eigenvalues and Eigenvectors

In dimensional form the state vector, fluxes, and source terms are defined as

\[
Q = \begin{pmatrix}
\rho \phi_l \\
\rho_g \phi_g \\
\rho u \\
\rho v \\
E \\
\phi_l
\end{pmatrix}, \quad f(Q) = \begin{pmatrix}
\rho \phi_l u \\
\rho_g \phi_g u + p \\
\rho u u + p \\
\rho u v \\
(E + p) u \\
0
\end{pmatrix}, \quad g(Q) = \begin{pmatrix}
\rho \phi_l v \\
\rho_g \phi_g v + p \\
\rho v v + p \\
\rho v u \\
(E + p) v \\
0
\end{pmatrix}
\] (2.78)

\[
S_x = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma \kappa \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma \kappa u & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad S_y = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma \kappa \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma \kappa v \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\] (2.79)

where a compact matrix-vector form of the governing equations (Eqs. 2.1a-2.1e) is

\[
\frac{\partial Q}{\partial t} + A(Q) \frac{\partial Q}{\partial x} + B(Q) \frac{\partial Q}{\partial y} = S_x \frac{\partial Q}{\partial x} + S_y \frac{\partial Q}{\partial y}.
\] (2.80)

Assuming spatially and temporally frozen curvature [23], this system can be written in terms of the primitive variables \( V = (\rho \phi_l, \rho_g \phi_g, u, v, p, \phi_l)^T \) in quasi-linear form as

\[
\frac{\partial V}{\partial t} + A(V) \frac{\partial V}{\partial x} + B(V) \frac{\partial V}{\partial y} = 0
\] (2.81)
where the Jacobian matrices are defined as

\[
A(V) = \frac{\partial V}{\partial Q} \left( \frac{\partial f(Q)}{\partial Q} - S_x \right) \frac{\partial Q}{\partial V}, \tag{2.82}
\]

\[
B(V) = \frac{\partial V}{\partial Q} \left( \frac{\partial g(Q)}{\partial Q} - S_y \right) \frac{\partial Q}{\partial V}, \tag{2.83}
\]

\[
\frac{\partial Q}{\partial V} = \left( \frac{\partial V}{\partial Q} \right)^{-1}. \tag{2.84}
\]

The HLLC solver is applied on a direction by direction basis so the conditions along the \(x\) direction are examined noting that conditions along the \(y\) direction can be similarly derived.

The eigenvalues \(\Lambda_A\) and right eigenvector \(Q_A\) associated with the Jacobian \(A = Q_A \Lambda_A Q_A^{-1}\) are:

\[
Q_A = \begin{pmatrix}
\frac{-\rho_1 \phi_l}{c} & 1 & 0 & 0 & 0 & \frac{\rho_1 \phi_l}{c} \\
\frac{-\rho_g \phi_g}{c} & 0 & 1 & 0 & 0 & \frac{\rho_g \phi_g}{c} \\
1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 \\
-\rho c & 0 & 0 & \sigma \kappa & \rho c & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
\end{pmatrix}, \quad \Lambda_A = \begin{pmatrix}
u - c & 0 & 0 & 0 & 0 & 0 \\
0 & u & 0 & 0 & 0 & 0 \\
0 & 0 & u & 0 & 0 & 0 \\
0 & 0 & 0 & u & 0 & 0 \\
0 & 0 & 0 & 0 & u & 0 \\
0 & 0 & 0 & 0 & 0 & u + c \\
\end{pmatrix}. \tag{2.85}
\]

The eigenvalues are identical to the standard Euler system without surface tension and with a full set of eigenvectors the model is hyperbolic. Note surface tension terms do appear in the eigenvectors which account for the surface tension induced pressure jump across the material contact denoted by Eq. 2.38.
CHAPTER 3. AN INTERFACE CAPTURING SCHEME FOR MODELING ATOMIZATION IN COMPRESSIBLE FLOWS

A paper submitted to the Journal of Computational Physics

Daniel P. Garrick\textsuperscript{1}, Wyatt A. Hagen\textsuperscript{2}, & Jonathan D. Regele\textsuperscript{3}

Abstract

The study of atomization in supersonic flow is critical to ensuring reliable ignition of scramjet combustors under startup conditions. Numerical methods incorporating surface tension effects have largely focused on the incompressible regime as most atomization applications occur at low Mach numbers. Simulating surface tension effects in compressible flow requires robust numerical methods that can handle discontinuities caused by both shocks and material interfaces with high density ratios. In this work, a shock and interface capturing scheme is developed that uses the Harten-Lax-van Leer-Contact (HLLC) Riemann solver while a Tangent of Hyperbola for INterface Capturing (THINC) interface reconstruction scheme retains the fluid immiscibility condition in the volume fraction and phasic densities in the context of the five equation model. The approach includes the effects of compressibility, surface tension, and molecular diffusion. One and two-dimensional benchmark problems demonstrate the desirable interface sharpening and conservation properties of the approach. Two and three-dimensional examples of primary atomization of a liquid jet in a Mach 2 crossflow and secondary atomization of a liquid droplet after its interaction with a shockwave demonstrate the robustness of the method.

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3.1 Introduction

The current research is motivated by the technical challenges involving liquid fuel in supersonic combustors. Efficient combustion requires sufficient penetration, mixing qualities, and atomization of the liquid [3]. Numerical modeling can supplement experimental insights in understanding the physical processes involved during atomization, especially in flow regimes or at length scales which are otherwise difficult or impossible to measure experimentally. As of yet, little numerical work has been performed on the effects of surface tension on the atomization process in supersonic crossflow.

There exists a wide array of numerical approaches for simulating interfacial multiphase flow. These include interface tracking via Arbitrary Lagrangian Eulerian (ALE) [26, 36, 38] or free-Lagrange methods [39, 40, 41], front-tracking [42, 43, 47] and ghost fluid methods [49], and level set [86, 87] or volume of fluid [69] interface capturing type methods. Such approaches can be broadly categorized into two groups based on their treatment of the interface. These are the sharp interface method (SIM) and the diffuse interface method (DIM) approaches, each with their own set of advantages and disadvantages.

The SIM approach is attractive in that it preserves the discontinuous nature of the interface including treatment of interfacial physics such as surface tension. In the context of compressible flows with surface tension effects, front-tracking [31, 32], unstructured ALE [26], and coupled level set volume of fluid [33] methods have been successfully utilized by various researchers. However SIM approaches are not always well suited to large interface deformations and can involve geometrically complex reconstructions, remeshing, or require special thermodynamic treatment at interfaces.

The DIM interface capturing approach naturally handles large topological changes in the interface and is straightforward to implement in multiple dimensions. The interface consists of a sharp but mesh representable profile. In the context of the five equation model, fluid mixture rules are applied in the interface region based on specific thermodynamic assumptions such as pressure and velocity equilibrium between components. Various approaches for incorporating surface tension effects into the compressible DIM framework have also been developed [23, 25,
The primary drawback of the DIM approach is that without special treatment the interface region grows over time via numerical diffusion. This can cause significant solution errors especially in the presence of strong shocks and high density ratios [27, 58].

In an attempt to fix this shortcoming of the DIM approach, a number of different interface sharpening schemes have been developed to maintain a consistent interface width throughout the simulation. One option is to utilize higher order WENO reconstruction [59, 60], however, even with the reduced numerical diffusion the interface will smear over long time periods. Shukla et al. [58] developed non-conservative compression operators for sharpening the volume fraction and phasic density fields according to the material interface. The compression was applied as a “post-processing” step to the primitive variables after each physical timestep. It was shown to significantly improve the results of shock interface interaction problems in the presence of high density and pressure ratios despite being discretely non-conservative. Tiwari et al. [63] developed a new model where the same compression operators were incorporated into the governing equations directly and applied to the conserved variables in a thermodynamically consistent manner during the physical timestepping procedure. Garrick et al. [88] also extended these concepts to account for surface tension effects during the compression procedure. However, the non-conservative nature of the approach means interfacial features that are not well resolved can be lost. Shukla [27] largely addressed this issue by exchanging the non-conservative compression operator with a constrained level set reinitialization equation [89], however this approach is also subject to some small conservation error and still requires a separate compression operator for the phasic densities. So et al. [62] developed an anti-diffusion approach designed to specifically and conservatively counter the numerical diffusion of the employed numerical method. However, the approach is specific to the discretization and diffusion properties of the underlying numerical scheme employed and may over-sharpen the interface in the presence of physical strain.

An alternative approach is the THINC (Tangent of Hyperbola for INterface Capturing) scheme first developed for incompressible flows [66]. The method is conservative, does not alter the governing equations, and can easily be coupled with higher order discretizations. Numerous researchers have built upon the concept for incompressible flows [90], use with unstructured
triangular and tetrahedral grids [91], enhancements for improved multi-dimensional reconstruction [82, 92, 93], and applications to droplet impact [94, 95]. Recently, compressible variants have been developed by Nonomura et al. [96] for the two fluid and by Shyue and Xiao [97] for the single fluid multicomponent flow models. The single fluid model utilized a wave propagation method and has been applied to investigate the shock front behavior of supersonic liquid jets injected into quiescent gas [98]. However, both compressible variants were demonstrated only with the Euler equations without capillary forces. Furthermore, the THINC procedure was used only to reconstruct the volume fraction. The two fluid approach in [96] does not require sharpening of other variables while the single fluid approach in [97] used the reconstructed volume fraction to extrapolate the remaining conservative variables across the interface in a thermodynamically consistent manner.

The objective of the present work is to develop a numerical approach capable of simulating liquid atomization in supersonic flows. This is achieved with extensions of the previous work by Garrick et al. [88] to include non-uniform grids and molecular diffusion terms as well as the replacement of a non-conservative interface compression/sharpening scheme with a THINC reconstruction procedure. A simple extension to the THINC procedure is developed so that both the volume fraction and phasic density are uniquely reconstructed across the interface in a manner applicable to a general finite volume scheme. The advantages of the present approach are demonstrated with several benchmark problems. This is followed by simulations of droplet and liquid jet atomization in high speed compressible crossflows. The simulations account for compressibility, surface tension, and molecular diffusion effects and demonstrate the robustness of the method.

The paper is organized as follows. Section 3.2 describes the governing equations and mixture rules. Section 3.3 discusses the overall spatial and temporal discretization and the interface normal and curvature computation. Section 3.4 introduces the proposed $\rho$-THINC reconstruction approach. Section 3.5 presents the results for a number of test cases involving atomization in compressible flows. These include the interaction of a liquid droplet with a shockwave and a liquid jet injected into a Mach 2 crossflow. This is followed with conclusions in Section 3.6.
3.2 Governing equations

A non-dimensional form of the quasi-conservative five equation model of Allaire [57] is employed with capillary and molecular diffusion terms. As such, the compressible multicomponent Navier-Stokes equations govern the flowfield [23]:

\[
\begin{align*}
\frac{\partial \rho_1 \phi_1}{\partial t} + \nabla \cdot (\rho_1 \phi_1 \mathbf{u}) &= 0, \\
\frac{\partial \rho_2 \phi_2}{\partial t} + \nabla \cdot (\rho_2 \phi_2 \mathbf{u}) &= 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) &= \frac{1}{Re_a} \nabla \cdot \mathbf{\tau} + \frac{1}{We_a} \kappa \nabla \phi_1, \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{u}) &= \frac{1}{Re_a} \nabla \cdot (\mathbf{\tau} \cdot \mathbf{u}) + \frac{1}{We_a} \kappa \nabla \phi_1 \cdot \mathbf{u}, \\
\frac{\partial \phi_1}{\partial t} + \mathbf{u} \cdot \nabla \phi_1 &= 0,
\end{align*}
\]

where \(\rho_1 \phi_1\), \(\rho_2 \phi_2\), and \(\rho\) are the liquid, gas, and total densities, \(\mathbf{u} = (u, v, w)^T\) is the velocity, \(\phi_1\) is the liquid volume fraction, \(p\) is the pressure, \(We_a\) and \(Re_a\) are the acoustic Weber and Reynolds numbers, respectively, \(\kappa\) is the interface curvature, and \(E\) is the total energy

\[
E = \rho e + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u}
\]

where \(e\) is the specific internal energy. The viscous stress tensor \(\mathbf{\tau}\) is given with the non-dimensional mixture viscosity \(\mu\):

\[
\mathbf{\tau} = 2\mu \left( \mathbf{D} - \frac{1}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right)
\]

where \(\mathbf{D}\) is the deformation rate tensor

\[
\mathbf{D} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T).
\]

The fluid components are considered immiscible and the liquid and gas volume fraction functions \((\phi_1\) and \(\phi_2\) respectively) are used to capture the fluid interface. Mass is discretely conserved for each phase via individual mass conservation equations. Surface tension is implemented as a volume force as in the CSF model [22] with terms in both the momentum and energy equations [23]. While a conservative form of the surface tension force exists [71], the present model utilizes the non-conservative form which enables flexible treatment of the curvature term \(\kappa\) and its accuracy. The model is non-dimensionalized using the rules in Table 3.1.
Table 3.1  Non-dimensional rules used in the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>$x = x'/l'_0$</td>
</tr>
<tr>
<td>Time</td>
<td>$t = t'a'_0/l'_0$</td>
</tr>
<tr>
<td>Velocity</td>
<td>$u = u'/a'_0$</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho = \rho'/\rho'_0$</td>
</tr>
<tr>
<td>Pressure</td>
<td>$p = p'/\rho'_0a'_0^2$</td>
</tr>
<tr>
<td>Total Energy</td>
<td>$E = E'/\rho'_0a'_0^2$</td>
</tr>
<tr>
<td>Curvature</td>
<td>$\kappa = \kappa'l'_0$</td>
</tr>
<tr>
<td>Surface tension coefficient</td>
<td>$\sigma = \frac{1}{We_a} = \frac{\sigma'_0}{\rho'_0a'_0^2}$</td>
</tr>
<tr>
<td>Viscosity</td>
<td>$\mu = \frac{1}{Re_a} = \frac{\mu'_0}{\rho'_0a'_0}$</td>
</tr>
</tbody>
</table>

where primes indicate dimensional quantities and the subscript ‘0’ refers to a chosen reference state. This results in the viscous and capillary forces being scaled by acoustic Reynolds and Weber numbers:

$$Re_a = \frac{\rho'_0a'_0^2}{\mu'_0} \quad (3.5)$$
$$We_a = \frac{\rho'_0a'_0^2}{\sigma'_0} \quad (3.6)$$

where $\mu'_0$ and $\sigma'_0$ are the reference dimensional viscosity and surface tension coefficients, respectively.

3.2.1 Mixture rules

The diffuse interface capturing approach results in the material interface being spread over several grid cells. In this diffuse region, the fluid is treated as a mixture that is neither purely gas nor liquid. Flow variables within this mixture region are defined as follows. The liquid (1) and gas (2) volume fractions are related by

$$\phi_2 = 1 - \phi_1. \quad (3.7)$$

The total density is given by

$$\rho = \rho_1\phi_1 + \rho_2\phi_2 \quad (3.8)$$

with internal energy

$$\rho e = \rho_1\phi_1e_1 + \rho_2\phi_2e_2. \quad (3.9)$$
Utilizing an isobaric assumption [57, 60] and the stiffened gas equation of state (EOS) [72]

\[ p = (\gamma - 1)\rho e - \gamma\pi_{\infty} \]  \hspace{1cm} (3.10)

the EOS parameters are given by

\[ \Gamma = \frac{1}{\gamma - 1} = \frac{\phi_2}{\gamma_2 - 1} + \frac{\phi_1}{\gamma_1 - 1}, \]  \hspace{1cm} (3.11)

\[ \Pi = \frac{\gamma\pi_{\infty}}{\gamma - 1} = \frac{\phi_2\gamma_2\pi_{\infty,2}}{\gamma_2 - 1} + \frac{\phi_1\gamma_1\pi_{\infty,1}}{\gamma_1 - 1}, \]  \hspace{1cm} (3.12)

such that the total energy can be written as

\[ E = \Gamma p + \Pi + \frac{1}{2}\rho \mathbf{u} \cdot \mathbf{u}. \]  \hspace{1cm} (3.13)

The isobaric assumption has been successfully employed in prior work to simulate surface tension in a compressible multicomponent framework [23, 25, 27, 70, 88]. The mixture speed of sound is given by

\[ c = \sqrt{\frac{\gamma(p + \pi_{\infty})}{\rho}} \]  \hspace{1cm} (3.14)

where the mixture quantities \( \gamma \) and \( \pi_{\infty} \) are computed using Eqs. 3.11 and 3.12. The mixture rules described above are applied throughout the domain but simplify to either the gas or liquid parameters outside the interface region. Similar to Coralic and Colonius [60], the mixture viscosity is determined following Perigaud and Saurel [23] but written in non-dimensional form for use in Eq. 3.3:

\[ \mu = \frac{\mu_1'}{\mu_0''} \phi_1 + \frac{\mu_2'}{\mu_0''} \phi_2 = N \phi_1 + \phi_2 \]  \hspace{1cm} (3.15)

where the liquid (1) and gas (2) viscosities are assumed to remain constant with the gas viscosity used as the reference state \( \mu_0' \). As a result, \( \mu_2'/\mu_0' = 1 \) and \( N = \mu_1'/\mu_0' \) becomes the liquid to gas viscosity ratio.

3.3 Numerical method

3.3.1 Spatial and temporal discretization

The numerical method is based on the work of Garrick et al. [88] where the effects of surface tension were incorporated into a compressible multicomponent framework. That model is
extended in the present work to three dimensions while accounting for molecular diffusion following the approach of Coralic and Colonius [60]. The final model (Eqs. 3.1a-3.1e) is discretized using the finite volume method on a non-uniform Cartesian grid. The resulting semi-discrete form of the equations is given for cell \((i, j, k)\) by:

\[
\frac{dQ_{i,j,k}}{dt} = -\frac{1}{\Delta x} \left[ (f_{i+1/2}^v - f_{i-1/2}^v) - \left( f_{i+1/2}^v - f_{i-1/2}^v \right) \right] \\
- \frac{1}{\Delta y} \left[ (g_{j+1/2}^v - g_{j-1/2}^v) - \left( g_{j+1/2}^v - g_{j-1/2}^v \right) \right] \\
- \frac{1}{\Delta z} \left[ (h_{k+1/2}^v - h_{k-1/2}^v) - \left( h_{k+1/2}^v - h_{k-1/2}^v \right) \right] + S_{i,j,k}
\]

\[
= R(Q_{i,j,k})
\]

(3.16)

where \(Q\) is the vector of state variables, \(f, g, h, \) and \(f^v, g^v, h^v\) are the conservative convective and viscous fluxes in the \(x\), \(y\), and \(z\) directions respectively, \(S_{i,j,k}\) is the source term, and \(R(Q_{i,j,k})\) is the residual function.

The convective fluxes are upwinded using the HLLC approximate Riemann solver [74, 75], i.e.

\[
f_{i-\frac{1}{2},j,k} = \hat{f}(Q^L_{i-\frac{1}{2},j,k}, Q^R_{i-\frac{1}{2},j,k})
\]

(3.17)

with modifications for surface tension by Garrick et al. [88] and described in Appendix A. To ensure oscillation free advection of material interfaces the HLLC solver features adaptations for a quasi-conservative form of the volume fraction transport equation following Johnsen and Colonius [59]. The left and right states \(Q^L, Q^R\) in Eq. 3.17 are determined via spatial reconstruction of the primitive variables. This reconstruction is performed using any suitable scheme such as WENO or MUSCL while the reconstructed volume fraction and phasic density for computational cells in the interfacial region, i.e. \((*)^L_{\frac{1}{2},j,k}, (*)^R_{\frac{1}{2},j,k}\) where \((*) = (\rho_1\phi_1, \rho_2\phi_2, \phi_1)\), are replaced with those values determined by the \(\rho\)-THINC scheme outlined in the following section.

Finally, velocity gradients \((\nabla \mathbf{u})\) for computation of viscous fluxes are computed following Coralic and Colonius [60]

\[
\frac{\partial u_{i,j,k}}{\partial x} = \frac{u_{i+1/2,j,k} - u_{i-1/2,j,k}}{\Delta x}.
\]

(3.18)
The conserved variables are then integrated in time using the following third order TVD Runge-Kutta scheme [73]:

\[
Q^{(1)}_{i,j,k} = Q^n_{i,j,k} + \Delta t R(Q^n_{i,j,k}),
\]

\[
Q^{(2)}_{i,j,k} = \frac{3}{4} Q^n_{i,j,k} + \frac{1}{4} Q^{(1)}_{i,j,k} + \frac{1}{4} \Delta t R(Q^{(1)}_{i,j,k}),
\]

\[
Q^{n+1}_{i,j,k} = \frac{1}{3} Q^n_{i,j,k} + \frac{2}{3} Q^{(2)}_{i,j,k} + \frac{2}{3} \Delta t R(Q^{(2)}_{i,j,k}).
\]

### 3.3.2 Interface normal and curvature computation

The interface normals are computed using a smoothed interface function [58]

\[
\psi = \frac{\phi_1}{\phi_1^{\alpha} + (1 - \phi_1)^{\alpha}}
\]

where \(\alpha = 0.1\). The normals are needed for the THINC reconstruction procedure even if surface tension terms are not included. If surface tension terms are included, the interface curvature is calculated via the interface normals

\[
\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \left( \frac{\nabla \psi}{|\nabla \psi|} \right).
\]

The vector quantity \(\nabla \psi\) and the curvature \(\kappa = -\nabla \cdot \mathbf{n}\) are calculated using second order central differences.

An interfacial (as opposed to spatial) filtering strategy is employed to locally improve the quality of the curvature calculation in the vicinity of the interface [88]. The \(m + 1\) value of curvature at cell \(i, j, k\) is corrected using weighted curvature values at iteration \(m\) by:

\[
\kappa_{i,j,k}^{m+1} = \frac{\sum_{l=1}^{27} w_l \kappa_l^m}{\sum_{l=1}^{27} w_l}
\]

with the weighting factor

\[
w_l = (\phi_{1,l}(1 - \phi_{1,l}))^2
\]

where \(\phi_{1,l}\) is the local volume fraction and \(l\) is a placeholder index corresponding to the different \((i, j, k)\) indices in the twenty-seven point stencil immediately surrounding the point \((i, j, k)\), i.e. \((i \pm 1, j \pm 1, k \pm 1)\), etc. The weighting factor is similar to the one used to interpolate curvature in the scheme of Renardy and Renardy [99]. The curvature is calculated and corrected at the
end of each physical timestep for use in the following timestep. The filtering strategy drives the curvature distribution within the diffuse interface region to the local value at \( \phi_1 = 0.5 \) which corresponds to the actual interface location if it were infinitely thin. For the surface tension related simulations demonstrated in this work, five iterations of the procedure are performed each time the curvature is computed.

### 3.4 The \( \rho \)-THINC reconstruction

A key aspect of multicomponent flow computation is the interface treatment. In the present work the volume fraction is used to specify which fluid occupies each computational cell (i.e. \( \phi_1 = 1 \) or \( \phi_1 = 0 \)). The location of the material interface is denoted as the region where the volume fraction falls between zero and one.

In order to maintain a set interface thickness with time, the THINC reconstruction procedure developed for incompressible flow by Xiao et al. [66] is employed. However, compressible flow means density variations can occur in the gas and liquid phases. As a result, a more general approach is developed to reconstruct the density jump across the interface. First, considering a one-dimensional case for cell \( i \), the THINC model assumes the volume fraction in grid cells encompassing the material interface will locally follow a hyperbolic tangent profile [96]:

\[
\phi_i(X) = \frac{1}{2} \left[ 1 + \tanh \left( \beta_i \left( \sigma_i X + x_{ic} \right) \right) \right]
\]  

where \( X \in [0,1] \) (3.24)

where the subscript 1 has been dropped from \( \phi \) for convenience, \( x_{ic} \) is the interface center, \( \sigma_i = \text{sgn}(\phi_{i+1,j,k} - \phi_{i-1,j,k}) \) is the sign of the volume fraction gradient, \( \beta_i \) determines the interface thickness, and \( X = \frac{x - x_{ic - 1/2}}{\Delta x} \). Note that with an appropriate choice of \( \beta_i \) such a hyperbolic tangent profile is identical to the steady state solution of the interface compression operators of Shukla et al. [58]. Following Xiao et al. [93], multidimensionality is accounted for by weighting \( \beta_i \) according to the interface orientation and the user specified slope parameter \( \beta \)

\[
\beta_i = \beta |n_{x,i}| + 0.01
\]  

where \( n_{x,i} \) is the \( x \) component of the interface normal \( \mathbf{n} \) with similar expressions in the \( y \) and \( z \) directions using \( n_y \) and \( n_z \). The interface center \( x_{ic} \) is the only unknown in Eq. 3.24 and can
be uniquely determined with the assumption that the cell average volume fraction for cell $i$ is represented by \[ \phi_i = \int_0^1 \phi_i(X) dX. \] (3.26)

The interface location is then given by
\[ x_{ic} = \frac{1}{2\beta_i} \ln \left( \frac{B - 1}{A - B} \right) \] (3.27)
where $A = \exp(2\sigma_i \beta_i)$ and $B = \exp(2\sigma_i \beta_i \phi_i)$. The left and right reconstructed volume fractions are then specified as
\[ \phi^{R}_{i-1/2} = \frac{1}{2} \left[ 1 + \tanh(\beta_i x_{ic}) \right], \] (3.28)
\[ \phi^{L}_{i+1/2} = \frac{1}{2} \left[ 1 + \tanh(\beta_i (\sigma_i + x_{ic})) \right]. \] (3.29)

The two fluid model utilized by Nonomura et al. [96] does not require sharpening of the other flow variables, however, the single fluid mixture model utilized in the present work and in the wave propagation method of Shyue and Xiao [97] requires a sharpening treatment for the phasic densities $\rho_1 \phi_1$ and $\rho_2 \phi_2$. Shyue and Xiao [97] followed So et al. [62] in determining the phasic densities via $\rho_k = \rho_k \phi_k / \phi_k$ for $k = 1, 2$. However, as noted by Tiwari et al. [63], determining $\rho_k$ in this manner could lead to spurious oscillatory behavior near the interface where both $\rho_k \phi_k$ and $\phi_k$ have large gradients. Instead, the present work extends the THINC reconstruction to the densities (hence $\rho$-THINC) by assuming the cell $i$ average phase density is represented by
\[ (\rho_1 \phi_1)_i = \rho_1,i \int_0^1 \phi_1,i(X) dX. \] (3.30)
This assumes that the phasic density profile $\rho_k \phi_k$ at the interface is driven primarily by the variation in $\phi_k$. A similar assumption (although not Eq. 3.30 specifically) has been used to derive the phasic density sharpening terms in other compressible interface sharpening schemes [58, 63]. As the interface location $x_{ic}$ has already been uniquely determined from Eq. 3.27, the only unknown in Eq. 3.30 is the phasic density $\rho_1$. A similar assumption for $\rho_2 \phi_2$ using $\phi_2 = 1 - \phi_1$ results in the expressions
\[ \rho_{1,i} = \frac{4\sigma_i \beta_i (\rho_1 \phi_1)_i}{E + 2\sigma_i \beta_i} \] (3.31)
\[ \rho_{2,i} = -\frac{4\sigma_i \beta_i (\rho_2 \phi_2)_i}{E - 2\sigma_i \beta_i} \] (3.32)
where

\[ E = \ln \left( \frac{(AD + 1)^2}{A(D + 1)^2} \right), \quad (3.33) \]

\( A = \exp(2\sigma_i\beta_i) \), and \( D = \exp(2\beta_i x_i) \). The left and right reconstructed phasic densities are then specified as

\[
\begin{align*}
(\rho_1\phi_1)^R_{i-1/2} &= \rho_{1,i} \phi_{i-1}^R, \\
(\rho_1\phi_1)^L_{i+1/2} &= \rho_{1,i} \phi_{i+1}^L, \\
(\rho_2\phi_2)^R_{i-1/2} &= \rho_{2,i} (1 - \phi_{i-1}^R), \\
(\rho_2\phi_2)^L_{i+1/2} &= \rho_{2,i} (1 - \phi_{i+1}^L),
\end{align*}
\]

where \( \phi_{i-1/2}^R \) and \( \phi_{i+1/2}^L \) are given by Eqs. 3.28 and 3.29. The remaining primitive variables (velocity and pressure) are reconstructed using a standard reconstruction approach, i.e. MUSCL or WENO. This differs from the work of Shyue and Xiao [97] who developed a homogeneous-equilibrium-consistent reconstruction scheme for the remaining variables within the interface. In summary, the approach results in the phasic densities \( \rho_1 \) and \( \rho_2 \) being uniquely determined in a manner consistent with the hyperbolic tangent profile used in the THINC procedure. The procedure only modifies the reconstruction of the volume fraction and phasic densities to the cell faces and unlike the PDE-based compression schemes does not require an intermediate step or affect the conservation properties of the underlying solution procedure.

Finally, following Shyue and Xiao [97], the \( \rho \)-THINC reconstruction is applied in any computational cell containing the interface. This is defined as any cell satisfying the condition \( \epsilon < \phi_1 \leq 1 - \epsilon \) where \( \epsilon = 10^{-5} \) and a monotonicity constraint \((\phi_{i+1} - \phi_i)(\phi_i - \phi_{i-1}) > 0\). The procedure is performed on a dimension by dimension basis such that replacing the indices \( i \) with \( j \) or \( k \) yields the reconstruction along the \( y \) or \( z \) directions, respectively.

### 3.5 Results and discussion

Benchmark interface advection, shock-interface interaction, and underwater explosion problems are first simulated without surface tension or diffusion terms. These problems demonstrate the shock capturing and conservative interface sharpening properties of the present scheme. The
behavior of the model with surface tension and molecular diffusion is then examined with a parasitic currents test. This is followed with simulations of secondary (cylindrical water column) and primary (2D and 3D liquid jet) atomization in compressible crossflows with surface tension and molecular diffusion effects.

The present implementation of surface tension terms follows the approach of Garrick et al. [88] while the implementation of molecular diffusion terms directly follows the approach of Coralic and Colonius [60]. Further validation and verification of these aspects of the present model can be found in those references.

### 3.5.1 Stiff gas interface advection and droplet transport

The objective of this test problem is to a) check the ability of the method to maintain a sharp interface, b) examine the effect of the sharpness parameter $\beta$, and c) ensure spurious pressure or velocity oscillations are not generated at the interface. The velocity and pressure are initialized to unity while the density and fluid properties vary across the interface. The liquid properties correspond to that of water with $\gamma_1 = 4.4$, $\pi'_{\infty,1} = 6 \times 10^8$ Pa [100]. The simulation is run to $t = 2$ with periodic boundaries such that the interface returns to its initial position. The initial conditions and EOS parameters are non-dimensionalized with the reference state $\rho'_0 = 1$ kg/m$^3$ and $a'_0 = \sqrt{10^5}$ m/s and are given by

$$(\rho_1 \phi_1, \rho_2 \phi_2, u, p) = (1000 \phi_1, 1 - \phi_1, 0.5, 1)$$

with fluid properties $\gamma_1 = 4.4$, $\pi_{\infty,1} = 6000$, $\gamma_2 = 1.4$, $\pi_{\infty,2} = 0$. Following [58], the material interface is initialized with a hyperbolic tangent function, i.e.

$$\phi_1 = \frac{1}{2} \left[ 1.0 + \tanh \left( \frac{x}{h} \right) \right],$$

on a domain extending from $[-1, 1]$ with 50 grid points ($h = 0.04$).

Figure 3.1 depicts the initial conditions and the solution computed after advecting for one period using the interface compression operator in Ref. [58] and the present $\rho$-THINC reconstruction scheme with a steepness parameter $\beta = 1$. Both methods retain the initial thickness of the interface after one period of advection. The effect of the $\rho$-THINC steepness
Figure 3.1 Comparison of interface compression to \( \rho \)-THINC data with \( \beta = 1 \) after one advection period using 50 grid points.

Table 3.2 Maximum velocity and pressure error at \( t = 2 \) in the stiff gas interface advection test problem. No spurious oscillations are observed in any of the solution variables.

| Case               | \( \max|u - u_0| \)      | \( \max|p - p_0| \)      |
|--------------------|---------------------------|---------------------------|
| Standard           | \( 2.20 \times 10^{-14} \) | \( 1.07 \times 10^{-11} \) |
| Compression        | \( 5.00 \times 10^{-15} \) | \( 1.88 \times 10^{-11} \) |
| \( \rho \)-THINC \( \beta = 0.5 \) | \( 3.00 \times 10^{-14} \) | \( 7.92 \times 10^{-12} \) |
| \( \rho \)-THINC \( \beta = 1 \) | \( 6.99 \times 10^{-15} \) | \( 5.22 \times 10^{-12} \) |
| \( \rho \)-THINC \( \beta = 2 \) | \( 4.00 \times 10^{-15} \) | \( 7.43 \times 10^{-12} \) |

parameter \( \beta \) on the interface thickness is depicted in Figure 3.2 where the “standard” solution refers to the results computed without either interface compression or \( \rho \)-THINC reconstruction. No spurious oscillations are generated in any of the solution variables with the maximum velocity and pressure error outlined in Table 3.2. The steepness parameter \( \beta \) is kept at unity for the remaining simulations in the paper as it maintains the initial sharp but mesh representable interface profile.

A similar two-dimensional problem is utilized to determine the ability of the method in maintaining the shape of an advecting droplet. It consists of a circular droplet of diameter \( D \) advected horizontally at \((u, v) = (1, 0)\) without surface tension or viscous effects in a \( 5D \times 5D \) domain with periodic boundary conditions [101]. Figure 3.3 depicts the results after one advection period for several grid resolutions using the present \( \rho \)-THINC reconstruction in Figure 3.3(a) compared to interface compression using the compression operator in Ref. [58].
Figure 3.2  Effect of steepness parameter $\beta$ on $\rho$-THINC interface profile after one advection period using 50 grid points. Standard refers to a simulation without interface compression or $\rho$-THINC.

and Figure 3.3(b). The non-conservative property of the interface compression scheme is especially evident at low grid resolutions where the $D/10$ grid resulted in total loss of the droplet after a single advection period. As a result, Figure 3.3(b) depicts the shape distortion without any interface treatment at the $D/10$ resolution while the $D/20$ and $D/40$ resolutions depict the results with interface compression. Meanwhile, Figure 3.3(a) shows significantly less variation between the different grid resolutions with the $\rho$-THINC scheme.

3.5.2 Shock-interface interaction

This test problem demonstrates the ability of the $\rho$-THINC method in computing accurate solutions of a shock-interface interaction. As noted by Coralic and Colonius [60], the position and speed of waves resulting from an interaction between a shockwave and an interface are commonly miscalculated by schemes which are discretely non-conservative at the interface. The initial conditions are a modified form of the problem studied by Liu et al. [52] and are given in non-dimensional form by [60, 102]:

$$
(\rho_1 \phi_1, \rho_2 \phi_2, u, p, \phi_1) = \begin{cases} 
(0.386, 0, 26.59, 100, 1) & \text{for } -1 \leq x < -0.8, \\
(0.1, 0, -0.5, 1, 1) & \text{for } -0.8 \leq x < -0.2, \\
(0, 1, -0.5, 1, 0) & \text{for } -0.2 \leq x \leq 1.
\end{cases} 
$$

(3.40)
Figure 3.3  Iso-lines of $\phi_1 = 0.5$ representing the gas-liquid interface after one advection period using (a) $\rho$-THINC compared to (b) interface compression using the compression operator in Ref. [58]. Plots show the exact solution (--) and numerical results with resolutions of $D/40$ (blue --), $D/20$ (red ---), and $D/10$ (green - -). For the $D/10$ resolution the results in (b) are computed without any interface treatment as the use of interface compression resulted in total loss of resolution of the droplet.

These conditions correspond to a helium-air interface at atmospheric pressure ($\gamma_1 = 1.67, \pi_{\infty,1} = 0, \gamma_2 = 1.4, \pi_{\infty,2} = 0$) traveling toward an oncoming Mach 8.96 shockwave originating in the helium.

The solution is evolved to the time $t = 0.07$ with adaptively chosen timesteps to meet a CFL restriction of 0.6. Figure 3.4 depicts the solution computed with 200 grid points using no interface treatment (“standard”), $\rho$-THINC interface reconstruction, and interface compression using the compression operator in Ref. [58]. Without interface treatment, the contact wave becomes smeared during the simulation. This is alleviated by both the $\rho$-THINC and interface compression approaches, however, the non-conservative nature of the interface compression scheme results in a small misprediction of the wave speeds. As a result, the locations of the reflected and transmitted waves are incorrect. This can be observed in the solution in Figure 3.4 and also in plots of the $L_1$ error for mixture density and total energy in Figure 3.5 on grids with 100, 200, 400, 800, 1600, and 3200 cells. As expected, in all cases the solution is no better than first order accurate due to the discontinuities, however, at each grid resolution the $\rho$-THINC scheme is observed to provide the most accurate results of the three approaches tested.
Figure 3.4 Comparison of results at $t = 0.07$ using the standard interface capturing scheme (◦) to those with interface compression (blue ×), $\rho$-THINC (red ▽), and the exact solution (−) on 200 grid points.

Figure 3.5 Mixture density and total energy error in the shock interface interaction problem for the standard interface capturing scheme (◦), interface compression (blue ×), $\rho$-THINC (red ▽).
3.5.3 Underwater explosion

An underwater explosion problem [27, 58, 85, 103, 104] is employed to test the conservation properties of the shock and interface capturing scheme. Static ambient atmospheric conditions are assumed for an air-water interface located at \( y = 0 \) with a circular pocket of highly compressed air at \( y = -0.3 \) with radius \( r = 0.12 \). The initial conditions are

\[
(\rho_1\phi_1, \rho_2\phi_2, u, v, p) =
\begin{cases}
(0, 1.225, 0, 0, 1.01325) & y > 0 \\
(0, 1250, 0, 0, 10^4) & r < 0.12 \\
(1000, 0, 0, 0, 1.01325) & \text{otherwise}
\end{cases}
\]

(3.41)

where \( r = \sqrt{x^2 + (y + 0.3)^2} \). To allow straightforward computation of the energy and mass conservation of the scheme all four boundaries are modeled as reflecting walls with no outflow. This does not noticeably change the overall interface dynamics of the problem which consists of a large topological change as the air bubble blasts upward through the surface.

Figure 3.6 depicts the solutions with the standard interface capturing scheme, the interface compression operator in Ref. [58], and \( \rho \)-THINC reconstruction at a solution time of 1.9 ms. A fluid ligament is formed separating the exploding air bubble from the atmosphere. As observed in previous work [27, 58], the non-conservative compression scheme results in the disappearance of this ligament without significant grid refinement. Similar ligament structures are a common feature during liquid atomization. The standard approach preserves the ligament but allows it to become significantly diffused leading to an underprediction of the bubble height as observed in Figure 3.6(a), and most evident at the lowest resolution. On the other hand, the \( \rho \)-THINC approach maintains a thin interface throughout the simulation and preserves the ligament structure while maintaining conservation. The global conservation of the mixture density and total energy for the different approaches are detailed in Tables 3.3 and 3.4. Both the standard and \( \rho \)-THINC approach conserve mass and energy to machine precision while the interface compression scheme exhibits losses in both.
Figure 3.6 Contours of liquid volume fraction for the underwater explosion problem at \( t = 1.9 \) ms.

Table 3.3 Conservation of mass (\( \mathcal{M} = \int \rho dV \)) measured by \( \left| \mathcal{M}_{\text{initial}} - \mathcal{M}_{\text{final}} \right| / \mathcal{M}_{\text{initial}} \) for the underwater explosion problem at \( t = 1.9 \text{ms} \).

<table>
<thead>
<tr>
<th>Grid</th>
<th>( \rho )-THINC</th>
<th>Standard</th>
<th>Compression</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 \times 300</td>
<td>1.52 \times 10^{-13}</td>
<td>1.31 \times 10^{-13}</td>
<td>1.06 \times 10^{-2}</td>
</tr>
<tr>
<td>600 \times 600</td>
<td>5.68 \times 10^{-13}</td>
<td>5.18 \times 10^{-13}</td>
<td>5.80 \times 10^{-3}</td>
</tr>
<tr>
<td>1200 \times 1200</td>
<td>6.50 \times 10^{-13}</td>
<td>4.70 \times 10^{-13}</td>
<td>3.82 \times 10^{-4}</td>
</tr>
</tbody>
</table>

Table 3.4 Conservation of energy (\( \mathcal{E} = \int E dV \)) measured by \( \left| \mathcal{E}_{\text{initial}} - \mathcal{E}_{\text{final}} \right| / \mathcal{E}_{\text{initial}} \) for the underwater explosion problem at \( t = 1.9 \text{ms} \).

<table>
<thead>
<tr>
<th>Grid</th>
<th>( \rho )-THINC</th>
<th>Standard</th>
<th>Compression</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 \times 300</td>
<td>2.10 \times 10^{-13}</td>
<td>1.78 \times 10^{-13}</td>
<td>1.49 \times 10^{-2}</td>
</tr>
<tr>
<td>600 \times 600</td>
<td>4.78 \times 10^{-13}</td>
<td>4.30 \times 10^{-13}</td>
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<tr>
<td>1200 \times 1200</td>
<td>2.42 \times 10^{-12}</td>
<td>2.43 \times 10^{-12}</td>
<td>9.92 \times 10^{-4}</td>
</tr>
</tbody>
</table>
### 3.5.4 Parasitic currents

Spurious velocities can be generated when surface tension is included due to errors in the calculation of the interface curvature and the competition between viscous and capillary forces \[20, 23, 79, 80\]. Even though the practical applications of the present work are in the high speed compressible regime, the common test case of a static droplet (i.e. \( M \approx 0 \)) is used to evaluate the parasitic currents of the present scheme. If all forces are equally balanced the droplet should remain stationary with zero velocity and the Laplace law (pressure jump due to surface tension) should be satisfied. Previous work \[88\] using the Euler equations verified that the present implementation of surface tension satisfies the Laplace law to within machine precision with no spurious velocities if the exact curvature is provided. Additionally, it showed the parasitic currents stayed within reasonable magnitudes when utilizing an interface compression scheme and numerically computed curvature using the procedure described in Section 3.3.2. The present method will extend this analysis with the inclusion of molecular diffusion terms and with the proposed \( \rho \)-THINC interface reconstruction scheme rather than interface compression.

The effect of the parasitic currents are reported in terms of the capillary number measured as \( Ca = |u'|_{max} \mu' / \sigma' = |u|_{max} We_a / Re_a \) where primes denote the dimensional quantities. Simulations are characterized by the Laplace number \( La = 1 / Oh^2 \) where larger values generally correspond to greater numerical difficulty. For a simulation with density ratio \( \epsilon \), viscosity ratio \( N \), and acoustic Weber and Reynolds numbers \( We_a \) and \( Re_a \), the Ohnesorge number is uniquely determined by \( Oh = (N/Re_a) \sqrt{We_a/\epsilon} \). Following Chang et al. \[32\] and Luo et al. \[35\] the initial conditions consist of a static liquid droplet in air with density ratio \( \epsilon = 1000 \), viscosity ratio \( N = 1 \), and unity diameter (\( D = 1 \)). The non-dimensionalization and EOS parameters are given as in the stiff gas interface advection problem in Section 3.5.1. The interface is initialized in a slightly diffused state as in the interface advection problem:

\[
\phi_1 = \frac{1}{2} \left[ 1 - \tanh \left( \frac{r - 1/2}{h} \right) \right] \tag{3.42}
\]

with \( r = \sqrt{x^2 + y^2} \) and constant grid spacing \( \Delta x = \Delta y = h \) on a \([-1,1] \times [-1,1] \) domain with no-slip boundary conditions.
Table 3.5 Capillary number for various conditions on different grid resolutions.

<table>
<thead>
<tr>
<th>La = 1/Oh^2</th>
<th>Re_a/We_a</th>
<th>20 × 20</th>
<th>40 × 40</th>
<th>80 × 80</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^6</td>
<td>10^2/10^1</td>
<td>2.29 × 10^{-5}</td>
<td>2.23 × 10^{-5}</td>
<td>2.70 × 10^{-5}</td>
</tr>
<tr>
<td>10^7</td>
<td>10^2/10^0</td>
<td>1.71 × 10^{-5}</td>
<td>2.27 × 10^{-5}</td>
<td>2.63 × 10^{-5}</td>
</tr>
<tr>
<td>10^7</td>
<td>10^3/10^2</td>
<td>3.31 × 10^{-6}</td>
<td>3.57 × 10^{-6}</td>
<td>4.66 × 10^{-6}</td>
</tr>
<tr>
<td>10^{11}</td>
<td>10^4/10^0</td>
<td>2.41 × 10^{-7}</td>
<td>3.88 × 10^{-7}</td>
<td>4.60 × 10^{-7}</td>
</tr>
</tbody>
</table>

Figure 3.7 Initial interface state (a) compared to results at t = 25 in (b) and velocity vectors in (c) for the extreme case of La = 1 × 10^{11} on an 80 × 80 grid. The black contour lines on either side of the interface mark the φ_1 = 0.01, 0.99 cutoff.

Laplace numbers of 10^6, 10^7, and 10^{11} are simulated by varying the acoustic Weber and Reynolds numbers. Simulations are performed to a non-dimensional solution time of t = 25. The corresponding non-dimensional time given by t'σ'/(µ'D') = tRe_a/(We_aD) varies from 250 to 250,000 for the various cases tested. Note that for the most extreme cases tested with an acoustic Weber number of unity the surface tension induced pressure jump across the interface is twice the magnitude of the ambient pressure in the simulation.

Table 3.5 lists the capillary number at the end of the simulations for a number of different grid resolutions and Laplace numbers. Figure 3.8 depicts the capillary number over time for the three grid resolutions tested. The droplet interface φ_1 = 0.5 iso-line remains stable even for the simulation with La = 10^{11} which results in the highest magnitude of spurious velocities. However, in this extreme case a slight disturbance does appear in the φ_1 = 0.01 iso-line due to the interaction of the parasitic currents with the THINC reconstruction scheme as depicted...
in Figures 3.7(a) vs. 3.7(b). Overall, the trends appear to be consistent with the observations of parasitic currents in CSF and volume of fluid based simulations by Harvie et al. [79] with spurious velocities generally increasing with mesh refinement and lower Weber numbers. To the authors’ knowledge, the highest achievable Laplace numbers currently reported are in the range of $10^{10} - 10^{11}$ using interface tracking methods [32, 35], see [32] for a comprehensive summary. Importantly, practical applications of the present method will generally involve velocity scales several orders of magnitude larger than the spurious velocities observed in the parasitic currents.

### 3.5.5 Droplet-shock interaction and breakup

Significant research has been performed on secondary atomization of liquid droplets, most recently reviewed by Guildenbecher et al. [6]. Generally experimental work utilizes either a continuous air jet or a shock tube to induce aerobreakup of the droplets. Many incompressible numerical investigations of breakup have also been performed, for example [105, 106, 107, 108, 109, 110]. However, compressible simulations of droplet breakup to date neglected surface
tension and examined only the early stages of the shock-droplet interaction and deformation [15, 16, 27, 46, 47, 58, 96, 111].

The initial conditions consist of a $D = 1$ liquid droplet being impacted by a $M_s = 1.39$ shockwave in air:

\[
\begin{aligned}
(r_1\phi_1, r_2\phi_2, u, v, w, p, \phi_1) &= \\
(0, 1.672, 0.559, 0, 0, 1.491, 0) & \text{for } x \leq -1.5, \\
(1000\phi_1, 1 - \phi_1, 0, 0, 0, 1/1.4 + \Delta p, \phi_1) & \text{otherwise}
\end{aligned}
\]

(3.43)

where $\phi_1$ is defined similarly to the previous simulation and $\Delta p$ is the pressure jump in the droplet due to the surface tension. The remaining non-dimensional simulation parameters are set as follows: viscosity ratio $N = 45$, $\gamma_g = 1.4$, $\pi_{\infty,g} = 0$, $\gamma_l = 4.4$, $\pi_{\infty,l} = 6000/1.4$, $\text{Re}_a = 2140$, and $\text{We}_a = 28.7$. The initial pressure jump $\Delta p$ is dictated by the Laplace law and varies in two and three dimensions as $(\Delta p)_{2D} = \phi_1/(0.5\text{We}_a)$, and $(\Delta p)_{3D} = 2(\Delta p)_{2D}$ according to the exact two and three-dimensional curvature of the droplet and the surface tension coefficient. The two-dimensional domain extends from $[-10, 18] \times [0, 18]$ with a Dirichlet boundary upstream, a symmetry condition along $y_{min}$, and extrapolation boundaries elsewhere. Uniform grid spacing is used in the vicinity of the droplet corresponding to fifty points across the initial cell radius with cells stretching to the farfield boundaries. The post shock conditions are a Mach 0.5 crossflow. The acoustic Weber and Reynolds numbers are chosen such that the initial flow Weber and Reynolds numbers for the droplet will be approximately 15 and 2000 respectively. This corresponds to an Ohnesorge number of 0.0036. As the droplet is slowly accelerated by the flow and full breakup can occur over distances of up to 50-100 droplet diameters [112], additional computational efficiency is gained by translating the static domain with the $x$ component of the center of mass. This requires appropriate modifications to the fluxes via a simplified arbitrary Lagrangian Eulerian (ALE) formulation [36]. The liquid center of mass (and thus the moving grid) velocity $u_c$ is determined via [16]:

\[
u_c = \frac{\int r_1\phi_1 u dV}{\int r_1\phi_1 dV}.
\]

(3.44)
The individual control volumes remain static, however, the overall computational domain translates downstream such that the liquid center of mass remains approximately centered throughout the simulation allowing significantly longer simulations to be performed.

Figure 3.9 depicts a time history of the two-dimensional droplet. The interaction of the shock with the droplet does not noticeably disturb the gas-liquid interface. However, the induced crossflow behind the shockwave gradually deforms and flattens the droplet. A weak shock is observed in the recirculation (upstream jetting) region behind the droplet starting in Figure 3.9(f). A similar shock and upstream jetting is observed in the results of Terashima and Tryggvason [46] and noted by Meng and Colonius [16] where a comparable problem was simulated without surface tension effects.

In the present simulations, vortices are observed downstream of the droplet which interact with the gas-liquid interface leading to a small amount of liquid mass being stripped from the droplet surface. This mass coalesces into a number of small particles in Figure 3.9(d). These particles should not be considered physical droplets and involve only small volume fractions (i.e. \(<< 0.1\)) with sizes on the order of the grid spacing. Due to the high gas-liquid density ratio, their appearance is exaggerated in the numerical Schlieren which highlights density gradients. The coalescence of this stripped mass into circular particles is partly due to the “numerical surface tension” property associated with interface sharpening schemes and which occurs even in the absence of physical surface tension forces [113].

A unique backwards facing bag-and-stamen type structure is observed as the rim of the droplet is pushed downstream while a small piece at the center remains relatively flattened, possibly due to the presence of the downstream shock. Finally, the bag ruptures and generates numerous small droplets as depicted in Figure 3.9(i).

The three-dimensional case was simulated as a quarter droplet with symmetry boundary conditions. The domain extends from \([-3.5, 3.5] \times [0, 3] \times [0, 3]\) with a uniform grid spacing of \(h = 0.01\) in all three directions. The resulting grid consists of 63 million cells. Note that the proximity of the droplet to the boundary will undoubtedly have an effect on the results, however, it demonstrates the capability of the method in three dimensions. Additionally, as noted by Meng [114], the use of a Cartesian domain leads to grid-based deformation effects aligned
Figure 3.9  Time history of two-dimensional shock droplet-interaction and breakup. The non-dimensional solution time $t$ is scaled by the characteristic breakup time $t_c = \sqrt{\epsilon D/u}$ computed using post shock conditions. The top half of each image depicts numerical Schlieren with liquid volume fraction shown in pink. The bottom half shows pressure contours with a $\phi_1 = 0.5$ iso-line at the gas-liquid interface.
with the computational coordinate axes. Nevertheless, Figure 3.10 shows similar features exist between the two and three-dimensional cases. The reflected shock is observed in Figure 3.10(a) followed by deformation of the droplet into a pancake like shape. Then, a bag like structure begins forming where, as in the two-dimensional case, the outer rim gets swept back while a small area at the center of the droplet does not push through in Figures 3.10(e)-3.10(h). This is followed with a forwards facing bag forming in Figures 3.10(i) and 3.10(j) and followed by bag rupture.

3.5.6 Atomization of a liquid jet in a $M = 2$ crossflow

The development of liquid fuel supersonic combustion ramjets (scramjets) is a motivating factor for understanding liquid atomization in high speed crossflows. To date, numerical simulations in this flow regime utilized analytical, empirical, or subgrid models for modeling the breakup and atomization of the liquid jet, for example [8, 115, 116, 117, 118]. A notable exception is the recent large eddy simulations of Xiao et al. [33]

In order to demonstrate the capability of the developed numerical approach, a $D = 1$ liquid jet injected into a supersonic $M = 2$ crossflow is investigated in two and three dimensions. The acoustic Weber and Reynolds numbers are set to 20 and 500 and correspond to crossflow Weber and Reynolds numbers of 80 and 1000, respectively. Due to the computational expense of the three-dimensional simulation, the density ratio was set to $\epsilon = 100$. This allows a faster injection speed which was set to satisfy a liquid to gas momentum flux ratio $q = \rho_j u_j^2 / (\rho_g u_g^2)$ of 3.41. The $\pi_\infty$ term in the liquid EOS was also reduced by an order of magnitude such that the liquid sound speed is approximately the same as for $\epsilon = 1000$ and the liquid phase remains essentially incompressible. The non-dimensional parameters for the simulation are outlined in Table 3.6. A parabolic boundary layer profile is enforced with Dirichlet conditions at the inlet and thickness of $3D$. For the three-dimensional case, a symmetry boundary is employed on the inside spanwise boundary such that only half the jet is simulated. The bottom wall is set to no-slip and extrapolation conditions are enforced on the remaining boundaries. The two-dimensional domain extends from $[-5,30] \times [0,25]$ with a constant grid spacing $\Delta x = \Delta y = h = 0.02$ consisting of 50 grid points across the jet diameter which is centered at the
Figure 3.10 Time history of three-dimensional shock droplet-interaction and breakup from an oblique upstream view. The blue represents a $\phi_1 = 0.5$ iso-surface while the white is an iso-surface representation of a numerical Schlieren.
Table 3.6 Liquid jet simulation parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q )</td>
<td>3.41</td>
<td>( p )</td>
<td>1/1.4</td>
<td>( \gamma_l )</td>
<td>4.4</td>
</tr>
<tr>
<td>( \rho_g )</td>
<td>1</td>
<td>( N = \mu_l/\mu_g )</td>
<td>1</td>
<td>( \pi_{\infty,l} )</td>
<td>600/1.4</td>
</tr>
<tr>
<td>( u_g )</td>
<td>2</td>
<td>( \gamma_g )</td>
<td>1.4</td>
<td>( \mathrm{Re}_a )</td>
<td>500</td>
</tr>
<tr>
<td>( \rho_j )</td>
<td>100</td>
<td>( \pi_{\infty,g} )</td>
<td>0</td>
<td>( \mathrm{We}_a )</td>
<td>20</td>
</tr>
</tbody>
</table>

origin. This leads to an overall grid size of \(1750 \times 1250\) or approximately 2.2 million points. The three-dimensional domain extends from \([-5,30] \times [0,5] \times [0,15]\) with the same uniform grid spacing \(h = 0.02\). The resulting grid is \(1750 \times 250 \times 750\) or approximately 328 million grid points.

Figure 3.11 depicts a time history of the liquid jet in the two-dimensional simulation. A separation shock attached to the boundary layer rises and interacts with the bow shock induced by the presence of the liquid, creating a shear layer. Additionally, a recirculation region is observed just upstream of the liquid column. Very similar features were noted in the recent numerical simulations of Liu et al. [118] where a kinetic theory model was used for the droplet phase. Past \(t = 10.05\), gas entrainment can be observed on the upstream side of the liquid column where small droplets break off and enter the recirculation region. In the three-dimensional case flow can travel around the liquid column, however, the inherent blockage effects of a two-dimensional simulation leads to the creation of dramatic ligament and bag structures which are pulled downstream. These bag structures collide with the stripped droplets and break up further in Figure 3.12 resulting in the creation of a significant number of small droplets. This general behavior repeats periodically with new bag structures forming off the injected jet and traveling downstream where they breakup due to impact with other liquid structures or pinch off.

A time history of the three-dimensional simulation is shown in Figure 3.13. At the early stages, a bag structure is formed similar to the two-dimensional case. However, as the gas crossflow is able to travel around the three-dimensional liquid jet, the bag structures are less dramatic than those observed in the two-dimensional simulation. Instead, a periodic ripple effect is seen to develop on the liquid surface as it advects downstream. An effective Weber number can be computed behind the bow shock using the crossflow Mach and Weber numbers.
Figure 3.11  Time history of two-dimensional liquid jet injected into a $M = 2$ crossflow. Contours of velocity magnitude are depicted with liquid volume fraction shown in pink.
Figure 3.12  Time history of ligament breakup due to impact with stripped droplets in the two-dimensional simulation. Contours of velocity magnitude are depicted with liquid volume fraction shown in pink.
and the velocity and density normal shock relations [33]: \( We_{\text{eff}} = \frac{2+(\gamma-1)M^2}{(\gamma+1)M^2} \cdot We. \) For the present simulation, the effective Weber number and the wavelength of the observed surface instability non-dimensionalized by the jet diameter correlates well to the subsonic experimental data of Sallam et al. [119] as depicted in Figure 3.14. The surface waves also create small pockets of slow moving air above the liquid surface while high speed flow is observed underneath the jet. Far downstream, the bulk of the liquid does not continue penetrating significantly further into the crossflow. This behavior contrasts starkly with the two-dimensional case which due to blockage effects has lower flow speeds downstream of the injection point near the bottom wall. This caused a large bulk of liquid to be driven up into the crossflow. The three-dimensional simulation also exhibits complex shock structures emanating upward from the rippling liquid interface. A recirculation zone and a standing bow shock are observed on the upstream side of the injection point. The bow shock results in a localized high pressure zone on the front side of the jet as depicted in Figure 3.15.

Finally, negative pressures associated with the stiffened gas or Tait’s EOS for modeling the liquid phase have been noted by various researchers [29, 85, 100, 120, 121] and are generally attributed to the lack of either a cavitation or two fluid model in problems where liquid cavitation should occur. To prevent computational failure associated with this phenomenon without affecting the conservation properties of the method, the quantity \( p + \pi_\infty \) is enforced to remain above a small positive value, chosen as \( 10^{-9} \), when computing the speed of sound \( c = \sqrt{\gamma(p + \pi_\infty)/\rho}. \) Such a fix was necessary here to allow complete evolution of the liquid jet simulation to the desired time of \( t = 80. \)

### 3.6 Conclusion

A finite volume interface capturing method for simulating atomization in compressible flows is developed. The thickness of the gas liquid interface is maintained throughout the simulation by uniquely reconstructing both the volume fraction and phasic density using the \( \rho \)-THINC procedure. The procedure is simple to implement, does not modify the governing equations, and can easily handle the complex topological changes involved with atomization simulations.
Figure 3.13  Time history of three-dimensional liquid jet injected into a $M = 2$ crossflow. A slice at the centerline depicts contours of velocity magnitude with a 3D iso-surface representing the gas-liquid interface.
Figure 3.14  Wavelength of surface instability vs. effective Weber number with subsonic experimental data from Sallam et al. [119].

Figure 3.15  Gas-liquid interface in three-dimensional liquid jet simulation at $t = 40$. 
Additionally, it does not affect the conservation of the underlying numerical scheme or require specific modifications based on the diffusive properties of the discretization scheme employed. The approach is used to simulate two and three-dimensional liquid atomization in high speed compressible flows. In the droplet atomization case, the formation and rupture of a bag structure is observed. Complex flow features, interface deformation, and breakup feature prominently in both the two and three-dimensional liquid jet simulations. The robustness and potential applications of the approach opens significant avenues for further research in the context of liquid atomization in high speed flows.

3.7 Acknowledgments

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Appendix A: HLLC Solver

The numerical advective flux $f, g, h$ in the $x, y, z$ directions are upwinded with the HLLC Riemann solver. The fluxes and state vector $Q$ are given by

$$Q = \begin{pmatrix} \rho_1 \phi_1 \\ \rho_2 \phi_2 \\ \rho u \\ \rho v \\ \rho w \\ E \\ \phi_1 \end{pmatrix}, \quad f = \begin{pmatrix} \rho_1 \phi_1 u \\ \rho_2 \phi_2 u \\ \rho u + p \\ \rho v \\ \rho w + p \\ (E + p)u \\ \phi_1 u \end{pmatrix}, \quad g = \begin{pmatrix} \rho_1 \phi_1 v \\ \rho_2 \phi_2 v \\ \rho v + p \\ \rho w \\ \rho w + p \\ (E + p)v \\ \phi_1 v \end{pmatrix}, \quad h = \begin{pmatrix} \rho_1 \phi_1 w \\ \rho_2 \phi_2 w \\ \rho w + p \\ \rho w \\ (E + p)w \\ \phi_1 w \end{pmatrix}. \quad (3.45)$$
The viscous numerical flux is given by

\[
\begin{align*}
\mathbf{f}^v &= \begin{pmatrix} 0 \\ 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ \tau_{xx}u + \tau_{xy}v + \tau_{xz}w \\ 0 \end{pmatrix}, \\
\mathbf{g}^v &= \begin{pmatrix} 0 \\ 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ \tau_{yx}u + \tau_{yy}v + \tau_{yz}w \\ 0 \end{pmatrix}, \\
\mathbf{h}^v &= \begin{pmatrix} 0 \\ 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ \tau_{zx}u + \tau_{zy}v + \tau_{zz}w \\ 0 \end{pmatrix},
\end{align*}
\]

(3.46)

The final form of the HLLC flux is given compactly by [60]

\[
\hat{f} = \frac{1 + \text{sgn}(s_s)}{2} [\mathbf{f}_L + u_s(Q_{sL} - Q_L)] + \frac{1 - \text{sgn}(s_s)}{2} [\mathbf{f}_R + u_s(Q_{sR} - Q_R)]
\]

(3.47)

in conjunction with the intermediate state (for the \(x\) direction)

\[
Q_{sK} = \frac{s_K - u_K}{s_K - s_s} 
\begin{pmatrix} 
(\rho_1 \phi_1)_K \\
(\rho_2 \phi_2)_K \\
\rho_K s_s \\
\rho_K v_K \\
\rho_K w_K \\
E_K + (s_s - u_K) \left( \rho_K s_s + \frac{p_K - \sigma \kappa \phi_1}{s_K - u_K} \right) \\
\phi_1 
\end{pmatrix}
\]

(3.48)

where \(K = L, R\) refers to the left and right cell states and the curvature is defined here as

\[
\kappa = \frac{1}{2}(\kappa_L + \kappa_R)
\]

where \(\kappa_L\) and \(\kappa_R\) are the curvatures defined at the cell center of the left and
right cells, respectively. The wave speeds are computed using [76]

\[ s_- = \min(0, s_L), \quad s_+ = \max(0, s_R) \] (3.49)

where

\[ s_L = \min(\bar{\nu} - \bar{c}, u_L - c_L), \quad s_R = \max(\bar{\nu} + \bar{c}, u_L + c_L) \] (3.50)

where, following [60], \( \bar{\nu} = \frac{1}{2}(u_L + u_R) \) and \( \bar{c} = \frac{1}{2}(c_L + c_R) \). Note that far from the interface \((\phi_{1,R} - \phi_{1,L} = 0)\) or in the case of no surface tension \((\sigma = 0)\) this choice of wave speeds is identical to that of Batten et al. [77] but now accounts for surface tension effects near the interface [88]. Note that the HLLC solver is applied on a direction by direction basis and is straightforward to extend to multiple dimensions. Finally, the middle wave speed \( s_* \) is given by

\[ s_* = \frac{p_R - p_L + \rho_L u_L(s_L - u_L) - \rho_R u_R(s_R - u_R) - \sigma \kappa (\phi_{1,R} - \phi_{1,L})}{\rho_L(s_L - u_L) - \rho_R(s_R - u_R)} \] (3.51)

Following Johnsen and Colonius [59] the advection equation is written in quasi-conservative form

\[ \frac{\partial \phi_1}{\partial t} + \nabla \cdot (\phi_1 \mathbf{u}) = \phi_1 \nabla \cdot \mathbf{u} \] (3.52)

where the source term is evaluated within the \( i,j,k \) computational cell using

\[ (\phi_1 \mathbf{u})_{i,j,k} = (\phi_1)_{i,j,k} \left[ \frac{1}{\Delta x}(u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k}) + \frac{1}{\Delta y}(v_{i,j+\frac{1}{2},k} - v_{i,j-\frac{1}{2},k}) + \frac{1}{\Delta z}(w_{i,j,k+\frac{1}{2}} - w_{i,j,k-\frac{1}{2}}) \right] \] (3.53)

where the velocity at the face is determined from the HLLC solver by

\[ u_{i-\frac{1}{2},j,k} = \hat{u}(Q^L_{i-\frac{1}{2},j,k}, Q^R_{i-\frac{1}{2},j,k}) \] (3.54)

where

\[ \hat{u} = \frac{1 + \text{sgn}(s_*)}{2} \left[ u_L + s_- \left( \frac{s_L - u_L}{s_L - s_*} - 1 \right) \right] + \frac{1 - \text{sgn}(s_*)}{2} \left[ u_R + s_+ \left( \frac{s_R - u_R}{s_R - s_*} - 1 \right) \right] \] (3.55)

The remaining velocity components for the diffusive fluxes are determined by [60]:

\[ \hat{v} = \frac{1 + \text{sgn}(s_*)}{2} v_L + \frac{1 - \text{sgn}(s_*)}{2} v_R, \] (3.56)
\[ \hat{w} = \frac{1 + sgn(s_\ast)}{2} w_L + \frac{1 - sgn(s_\ast)}{2} w_R. \] (3.57)

For computation of viscous fluxes, the velocity gradient at the face is determined following Perigaud and Saurel [23] and Coralic and Colonius [60]

\[ \nabla \mathbf{u} = \frac{1}{2} [(\nabla \mathbf{u})_L + (\nabla \mathbf{u})_R] \] (3.58)

where the velocity gradients are determined in the \( x \) direction (and similarly in the \( y \) and \( z \) directions using \( j \pm \frac{1}{2} \) and \( k \pm \frac{1}{2} \) values) by

\[ \frac{\partial \mathbf{u}}{\partial x} = \frac{1}{\Delta x} (\mathbf{u}_{i+,1/2,j,k} - \mathbf{u}_{i-,1/2,j,k}). \] (3.59)

### 3.7.1 HLLC surface tension source terms

The present work includes additional modifications of the HLLC solver to account for the surface tension source terms [88]. For the surface tension force in the \( u \) momentum equation:

\[ \sigma \kappa \frac{\partial \phi}{\partial x} = \sigma \kappa_{i,j,k} \left[ \frac{1}{\Delta x} (\phi_{i+,1/2,j,k} - \phi_{i-,1/2,j,k}) \right] \] (3.60)

where the subscript 1 has been dropped from \( \phi \) for convenience. The force in the \( v \) and \( w \) momentum equations are treated similarly. For consistency, the velocity used in the source term should be the same as that used in the advective numerical flux [59, 60]. To achieve this, similarly to the advection equation, the surface tension source term in the energy equation is first decomposed into conservative and non-conservative terms using

\[ \nabla \cdot (\phi \mathbf{u}) = \phi \nabla \cdot \mathbf{u} + \nabla \phi \cdot \mathbf{u} \] (3.61)
such that

\[(\sigma \kappa \nabla \phi) \cdot \mathbf{u} = \sigma \kappa \left[ \nabla \cdot (\phi \mathbf{u}) - \phi \nabla \cdot \mathbf{u} \right] \quad (3.62)\]

\[
= \sigma \kappa_{i,j,k} \left[ \frac{1}{\Delta x} \left( (\phi u)_{i+\frac{1}{2},j,k} - (\phi u)_{i-\frac{1}{2},j,k} \right) 
+ \frac{1}{\Delta y} \left( (\phi v)_{i,j+\frac{1}{2},k} - (\phi v)_{i,j-\frac{1}{2},k} \right) 
+ \frac{1}{\Delta z} \left( (\phi w)_{i,j,k+\frac{1}{2}} - (\phi w)_{i,j,k-\frac{1}{2}} \right) 
- \phi_{i,j,k} \left( \frac{1}{\Delta x} \left( u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k} \right) 
+ \frac{1}{\Delta y} \left( v_{i,j+\frac{1}{2},k} - v_{i,j-\frac{1}{2},k} \right) 
+ \frac{1}{\Delta z} \left( w_{i,j,k+\frac{1}{2}} - w_{i,j,k-\frac{1}{2}} \right) \right) \right] \quad (3.63)\]

with

\[(\phi u)_{i+\frac{1}{2},j,k} = \phi_{i+\frac{1}{2},j,k} u_{i+\frac{1}{2},j,k}. \quad (3.64)\]

The face values are determined from the HLLC solver for the volume fraction by

\[
\phi = \frac{1 + sgn(s_s)}{2} \phi_L + \frac{1 - sgn(s_s)}{2} \phi_R, \quad (3.65)\]

and velocity by Eq. 3.55.
CHAPTER 4. NUMERICAL SIMULATIONS OF LIQUID COLUMN ATOMIZATION IN COMPRESSIBLE CROSSFLOWS

A paper to be submitted to Physical Review Fluids

Daniel P. Garrick\textsuperscript{1}, Wyatt A. Hagen\textsuperscript{2}, & Jonathan D. Regele\textsuperscript{3}

Abstract

To better understand the breakup behavior of water columns in supersonic flows, a range of Weber numbers are investigated for two shock Mach numbers consisting of either subsonic or supersonic post-shock conditions. The effects of compressibility, surface tension, and molecular diffusion are included. Fluid immiscibility is maintained with an interface sharpening scheme. In the subsonic case, a number of different breakup modes are observed with a strong dependence on the Weber number and provide good correlation with experimental observations, validating the approach. In the supersonic case, significantly less variation in the breakup behavior was observed across the same range of surface tension forces. In both cases, water columns at lower Weber numbers exhibit lower drag coefficients but less variation in the drag coefficient as a function of the Weber number is observed in the supersonic case.

4.1 Introduction

Liquid atomization is an important physical process in a wide variety of applications ranging from manufacturing to drug delivery to fuel sprays. The process of liquid breakup has a strong dependence on the Weber number which relates the inertial and surface tension forces. As a

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large quantity of atomization applications occur in low Mach number flow regimes, significant numerical modeling effort has focused on incompressible schemes [17]. Meanwhile, technical challenges involving supersonic combustion ramjets (scramjets) has identified a need for greater understanding of the penetration, mixing, and atomization of liquid jets injected into high-speed compressible crossflows [3].

Liquid jet atomization consists of primary and secondary breakup. The former consists of the bulk liquid transforming into smaller jets, sheets, and droplets. Secondary breakup consists of liquid droplets or ligaments undergoing further deformation and breakup and has generally been classified into vibrational, bag, multi-mode (or bag-and-stamen), sheet-thinning, and catastrophic regimes according to the Weber number [6, 68, 122, 123]. Simulating the entire atomization process requires extremely high resolution due to the multiscale nature of the features involved. This is especially problematic at high Reynolds and Weber numbers where large numbers of small droplets can be generated. Subgrid droplet models can relax the computational complexity and have been used to simulate liquid jet injection in supersonic crossflows [116, 118]. However they generally utilize steady-state empirical relations for the drag coefficient of solid spherical particles as a function of the particle Reynolds number to calculate drop trajectories [124].

To better understand the behavior of deforming droplets in crossflows and the secondary atomization process in general, various experimental and numerical studies have been performed and were recently reviewed by [6]. With respect to the drag coefficient, [125] found that the effects of the initial relative velocity and large relative acceleration or deceleration are significant when predicting rectilinear motion of spherical particles in crossflows. Experiments by [126] showed that the unsteady drag is always larger in decelerating or smaller in accelerating flows than the steady state value. Wadhwa et al. [127] coupled a compressible gas phase solver with an incompressible liquid phase solver and found for axisymmetric conditions the droplet Weber number affects the drag coefficient of a drop traveling at high speeds and placed in quiescent air. Finally, the unsteady nature of the flow as well as the scales (both temporal and spatial) involved in droplet breakup means experimentally measuring the local drop and ambient flow fields
during secondary atomization is incredibly challenging [6]. Therefore, numerical simulations are a valuable tool for providing important physical insight in such conditions.

Experimental investigation of liquid columns (as opposed to spherical droplets) allows for easier visualization of the wave structures [121, 128], although difficulties remain in visualizing the later stages of the breakup process. The deformation behavior of the liquid columns have also been found to follow similar trends as that of spherical droplets [111, 129]. Numerous researchers have simulated the two-dimensional shock-column interaction, commonly as a test case for compressible multicomponent flow solvers [15, 16, 27, 46, 47, 58, 96, 111]. Notable examples include [46] who simulated the entire evolution of the column break-up, while [16] and [15] examined the sheet-thinning process and evaluated column trajectories and drag coefficients. However, such studies focused on the early stages of breakup and neglected the effects of both surface tension and molecular diffusion. Additionally, both [16] and [15] utilized a diffuse interface model approach which is subject to numerical smearing of the gas-liquid interface. As a result, questions remain as to the break-up process of a liquid column when accounting for molecular diffusion and surface tension effects, especially in the context of supersonic flows.

To address this, the objective of the present work is to gain better understanding of the breakup process of liquid columns with a focus on the different behavior in subsonic versus supersonic flow conditions. This is achieved with detailed two-dimensional simulations of column breakup in compressible flows while accounting for capillary and viscous forces and utilizing an interface sharpening scheme to maintain the fluid immiscibility condition. The impact of the the Weber number and the Mach number on the column breakup process is examined along with the deformation behavior, drag coefficient, and flow characteristics around the column.

Garrick et al. [88] performed a preliminary study of a $M_s = 3$ shock column interaction without molecular diffusion and with and without surface tension forces together with a non-conservative interface sharpening scheme. This study considered only the early stages of breakup but successfully highlighted the effects of surface tension in combating column deformation. Garrick et al. [130] extended the method to account for molecular diffusion and non-uniform grids and replaced the non-conservative interface sharpening scheme with a conservative reconstruction based interface sharpening scheme. The model was then applied to
simulate primary and secondary atomization in high speed crossflow. The present work applies the model to a wider range of secondary atomization conditions.

The paper is organized as follows. Section 4.2 describes the mathematical model and non-dimensionalization. Section 4.3 describes the numerical approach while the problem statement is reviewed in Section 4.4. Section 4.5 presents the simulation results for a number of column breakup scenarios and examines the impact of surface tension on the column breakup, trajectory and drag coefficient, and flow characteristics. This is followed with conclusions in Section 4.6.

4.2 Mathematical model

The quasi-conservative five equation model of [57] is employed with capillary and molecular diffusion terms. As such, a non-dimensional form of the compressible multicomponent Navier-Stokes equations described by [23] govern the flowfield:

\[
\begin{align*}
\frac{\partial \rho_1 \phi_1}{\partial t} + \nabla \cdot (\rho_1 \phi_1 \mathbf{u}) &= 0, \\
\frac{\partial \rho_2 \phi_2}{\partial t} + \nabla \cdot (\rho_2 \phi_2 \mathbf{u}) &= 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) &= \frac{1}{\text{Re}_a} \nabla \cdot \mathbf{\tau} + \frac{1}{\text{We}_a} \kappa \nabla \phi_1, \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{u}) &= \frac{1}{\text{Re}_a} \nabla \cdot (\mathbf{\tau} \cdot \mathbf{u}) + \frac{1}{\text{We}_a} \kappa \nabla \phi_1 \cdot \mathbf{u}, \\
\frac{\partial \phi_1}{\partial t} + \mathbf{u} \cdot \nabla \phi_1 &= 0,
\end{align*}
\]

where \(\rho_1 \phi_1, \rho_2 \phi_2,\) and \(\rho\) are the liquid, gas, and total densities, \(\mathbf{u} = (u, v)^T\) is the velocity, \(\phi_1\) is the liquid volume fraction, \(p\) is the pressure, \(\text{We}_a\) and \(\text{Re}_a\) are the acoustic Weber and Reynolds numbers, respectively, \(\kappa\) is the interface curvature, and \(E\) is the total energy

\[E = \rho e + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u}\]

where \(e\) is the specific internal energy. The viscous stress tensor \(\mathbf{\tau}\) is given with the non-dimensional mixture viscosity \(\mu:\)

\[\mathbf{\tau} = 2\mu \left( \mathbf{D} - \frac{1}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right)\]

where \(\mathbf{D}\) is the deformation rate tensor

\[\mathbf{D} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) .\]
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>$x = x'/l'$</td>
</tr>
<tr>
<td>Time</td>
<td>$t = t'a_0/l'$</td>
</tr>
<tr>
<td>Velocity</td>
<td>$u = u'/a_0'$</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho = \rho'/\rho_0'$</td>
</tr>
<tr>
<td>Pressure</td>
<td>$p = p'/\rho_0a_0^2$</td>
</tr>
<tr>
<td>Total Energy</td>
<td>$E = E'/\rho_0a_0^2$</td>
</tr>
<tr>
<td>Curvature</td>
<td>$\kappa = \kappa'l'$</td>
</tr>
<tr>
<td>Surface tension coefficient</td>
<td>$\sigma = \frac{1}{We_a} = \frac{\sigma_0}{\rho_0a_0^2}$</td>
</tr>
<tr>
<td>Viscosity</td>
<td>$\mu = \frac{1}{Re_a} = \frac{\mu_0}{\rho_0a_0^2}$</td>
</tr>
</tbody>
</table>

The fluid components are considered immiscible and the liquid and gas volume fraction functions ($\phi_1$ and $\phi_2$ respectively) are used to capture the fluid interface. Mass is discretely conserved for each phase via individual mass conservation equations. Surface tension is implemented as a volume force using the CSF model of [22] with terms in both the momentum and energy equations [23]. While a conservative form of the surface tension force exists [71], the present model utilizes the non-conservative form which enables flexible treatment of the curvature term $\kappa$ and its accuracy. The model is non-dimensionalized using the rules in Table 4.1 where primes indicate dimensional quantities. This results in the viscous and capillary forces being scaled by acoustic Reynolds and Weber numbers:

$$Re_a = \frac{\rho_0a_0' l'}{\mu_0}$$

$$We_a = \frac{\rho_0a_0^2 l'}{\sigma_0}$$

where $\mu_0'$ and $\sigma_0'$ are the reference dimensional viscosity and surface tension coefficients, respectively.

### 4.2.1 Equation of state and mixture rules

To close the model, the stiffened gas equation of state [72] is employed to model both the gas and liquid phases. The equation of state parameters are given by

$$\Gamma = \frac{1}{\gamma - 1} = \frac{\phi_2}{\gamma_2 - 1} + \frac{\phi_1}{\gamma_1 - 1},$$
\[ \Pi = \frac{\gamma \pi_\infty}{\gamma - 1} = \frac{\phi_2 \gamma_2 \pi_\infty}{\gamma_2 - 1} + \frac{\phi_1 \gamma_1 \pi_\infty}{\gamma_1 - 1}, \]  
(4.8)

such that the total energy can be written as

\[ E = \Gamma p + \Pi + \frac{1}{2} \rho u \cdot u. \]  
(4.9)

The speed of sound is given by

\[ c = \sqrt{\frac{\gamma (p + \pi_\infty)}{\rho}} \]  
(4.10)

where the mixture quantities \( \gamma \) and \( \pi_\infty \) are computed using Eqs. 4.7 and 4.8. Similar to [60], the mixture viscosity is determined following [23] but written in non-dimensional form for use in Eq. 4.3:

\[ \mu = \frac{\mu'_1}{\mu'_0} \phi_1 + \frac{\mu'_2}{\mu'_0} \phi_2 \]
\[ = N \phi_1 + \phi_2 \]  
(4.11)

where the liquid (1) and gas (2) viscosities are assumed to remain constant with the gas viscosity used as the reference state \( \mu'_0 \). As a result, \( \mu'_2/\mu'_0 = 1 \) and \( N = \mu'_1/\mu'_0 \) becomes the liquid to gas viscosity ratio.

### 4.3 Numerical method

The model (Eqs. 4.1a-4.1e) is discretized using a finite volume method on a non-uniform two-dimensional Cartesian grid. The resulting semi-discrete form of the equations is given for cell \((i,j)\) by:

\[ \frac{dQ_{i,j}}{dt} = -\frac{1}{\Delta x} \left[ (f_{i+1/2} - f_{i-1/2}) - \left( f^v_{i+1/2} - f^v_{i-1/2} \right) \right] \\
- \frac{1}{\Delta y} \left[ (g_{j+1/2} - g_{j-1/2}) - \left( g^v_{j+1/2} - g^v_{j-1/2} \right) \right] + S_{i,j} \\
= R(Q_{i,j}) \]  
(4.12)

where \( Q \) is the vector of state variables, \( f, g, f^v, \) and \( g^v \) are the conservative convective and viscous fluxes in the \( x \) and \( y \) directions respectively, \( S_{i,j} \) is the source term, and \( R(Q_{i,j}) \) is the residual function.
The convective fluxes are upwinded using the Harten-Lax-van Leer-Contact (HLLC) approximate Riemann solver originally developed by Toro et al. [74, 75] with modifications for surface tension by Garrick et al. [88]. Following the approach of Johnsen and Colonius [59], oscillation free advection of material interfaces is ensured with adaptations to the HLLC for a quasi-conservative form of the volume fraction transport equation. Viscous terms are implemented following Coralic and Colonius [60]. Spatial reconstruction to cell faces is performed on the primitive variables using the second order MUSCL scheme with the minmod limiter. The fluid immiscibility condition is maintained using the \( \rho \)-THINC interface sharpening procedure [130] for reconstructing the phasic densities and volume fraction within the interface.

The conserved variables are then integrated in time using the following third order TVD Runge-Kutta scheme [73]:

\[
\begin{align*}
Q_{i,j}^{(1)} &= Q_{i,j}^n + \Delta t R(Q_{i,j}^n), \\
Q_{i,j}^{(2)} &= \frac{3}{4} Q_{i,j}^n + \frac{1}{4} Q_{i,j}^{(1)} + \frac{1}{4} \Delta t R(Q_{i,j}^{(1)}), \\
Q_{i,j}^{n+1} &= \frac{1}{3} Q_{i,j}^n + \frac{2}{3} Q_{i,j}^{(2)} + \frac{2}{3} \Delta t R(Q_{i,j}^{(2)}).
\end{align*}
\]

### 4.3.1 Interface normal and curvature computation

Interface curvature is calculated via the interface normals

\[
\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \left( \frac{\nabla \psi}{|\nabla \psi|} \right)
\]

where \( \psi \) is a smoothed interface function [58]

\[
\psi = \frac{\phi_l^\alpha}{\phi_l^\alpha + (1 - \phi_l)^\alpha}
\]

where \( \alpha = 0.1 \). The vector quantity \( \nabla \psi \) and the curvature \( \kappa = -\nabla \cdot \mathbf{n} \) are calculated using second order central differences. The present work also incorporates an interfacial (as opposed to spatial) filtering strategy to locally extend the value of the curvature at the center of the interface outward [88].
4.3.2 Water column attached domain

Additional computational efficiency is gained by translating the static domain with the \( x \) component of the column center of mass. This requires appropriate modifications to the fluxes via a simplified arbitrary Lagrangian Eulerian (ALE) formulation [36]. The liquid center of mass (and thus the moving grid) velocity \( u_c \) is determined via [16]:

\[
{u_c} = \frac{\int \rho_1 \phi_1 u dV}{\int \rho_1 \phi_1 dV}.
\]

(4.16)

The individual control volumes remain static, however, the overall computational domain translates downstream such that the liquid center of mass remains approximately centered throughout the simulation.

4.4 Problem statement

Standard benchmark cases to verify and validate the shock and interface capturing scheme and the implementation of surface tension were performed by Garrick et al. [88, 130]. For the present simulations, the initial conditions are depicted in Figure 4.1 and correspond to a liquid column (\( \rho_l = 1000 \) kg/m\(^3\)) in air (\( \rho_g = 1.2 \) kg/m\(^3\)) at ambient pressure (\( p = 101325 \) Pa). The column has unity non-dimensional diameter and is centered on the \( y \) minimum boundary of the domain. For computational efficiency symmetry conditions are enforced along this boundary. Dirichlet and extrapolation conditions are enforced on the upstream and remaining boundaries respectively. The domain consists of a block of uniform cells in the vicinity of the column corresponding to a resolution of 120 points across the initial column diameter. Grid stretching to the boundary results in an overall domain of 1579 × 795 cells.
Cases with shock Mach numbers of $M_s = 1.47$ and $M_s = 2.5$ are simulated with corresponding post-shock flow Mach numbers of $M = 0.58$ and $M = 1.2$. The acoustic Weber number was varied with values of 5, 10, 20, 50, and 100. The acoustic Reynolds number was held constant with a value of 1000 and a liquid to gas viscosity ratio of $N = \mu_l/\mu_g = 45$. In the dimensional sense, for a given surface tension coefficient, this corresponds to simulations of five different column diameters subjected to the two shock speeds. The primary purpose of the subsonic simulations is to verify the model qualitatively reproduces the various atomization modes as a function of the Weber number. The supersonic cases are then used to examine in detail what happens when columns of the same diameter as the subsonic cases are subjected to a higher incident shock speed.

The acoustic Weber number is given in terms of the reference quantities used to non-dimensionalize the system:

$$W_{ea} = \frac{\rho'_0 a'_0^2 d'_0}{\sigma'_0}.$$  \hspace{1cm} (4.17)

Meanwhile the crossflow Weber number corresponds to the local flow conditions at the column:

$$W_e = W_{ea} \rho (u - u_c)^2$$  \hspace{1cm} (4.18)

where $u$ and $u_c$ are the non-dimensional streamwise flow and column speed, respectively, such that $u - u_c$ is the relative velocity seen by the column and $\rho$ is the non-dimensional density behind the incident shockwave. The initial crossflow Weber number for each simulation can be estimated by scaling the acoustic Weber numbers by the initial post-shock conditions. These estimates are provided for the present simulations in Table 4.2. The initial crossflow Reynolds number is similarly estimated as $Re_{1.47} = 1430$ and $Re_{2.5} = 7000$ for the $M_s = 1.47$ and $M_s = 2.5$ cases respectively. In the supersonic case, an effective Weber number can also be estimated behind the bow shock using the crossflow Mach and Weber numbers and the velocity and density normal shock relations [33]: $W_{eff} = \frac{2+(\gamma-1)M^2}{(\gamma+1)M^2} W_e$. These values are also enumerated for the supersonic case in Table 4.2. Based on the crossflow Reynolds and Weber numbers, these simulations correspond to Ohnesorge numbers ranging from 0.003 to 0.014. Finally, simulation times are scaled into the non-dimensional characteristic time given by [67]:

$$t^* = \frac{tu}{Du \sqrt{\epsilon}}$$  \hspace{1cm} (4.19)
Table 4.2  Crossflow and effective Weber number estimates for the $M_s = 1.47$ and $M_s = 2.5$ simulations.

<table>
<thead>
<tr>
<th>$W_e$</th>
<th>$W_{e, 1.47}$</th>
<th>$W_{e, 2.5}$</th>
<th>$W_{e, eff, 2.5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>4.7</td>
<td>61</td>
<td>46</td>
</tr>
<tr>
<td>10</td>
<td>9.4</td>
<td>122</td>
<td>92</td>
</tr>
<tr>
<td>20</td>
<td>19</td>
<td>245</td>
<td>183</td>
</tr>
<tr>
<td>50</td>
<td>47</td>
<td>612</td>
<td>458</td>
</tr>
<tr>
<td>100</td>
<td>94</td>
<td>1225</td>
<td>917</td>
</tr>
</tbody>
</table>

where $u$ is the velocity and $\epsilon$ is the liquid to gas density ratio using the post-shock conditions.

4.5 Results and discussion

4.5.1 Flow characteristics

Figure 4.2 depicts a time history of the $W_{e, a} = 20$ case with a shock Mach number of $M_s = 1.47$. The top half of each image depicts the numerical Schlieren or normalized exponentially spaced density gradient [131] with liquid volume fraction in pink while the bottom half shows pressure contours. Figure 4.2(a) depicts the time period shortly after the incident shockwave has impacted the water column. This results in a transmitted shock traveling through the column and a circular reflected shockwave which propagates away from the column, as observed in Figure 4.2(b). The crossflow induced by the passage of the shockwave leads to continued deformation of the column in Figures 4.2(c)-4.2(f). Downstream of the column, a recirculation region is observed to form and grow in size in Figures 4.2(c)-4.2(e) where an upstream jet is observed. As the speed of this upstream jet reaches locally supersonic levels, a standing shock appears downstream of the column and grows in size beginning in Figures 4.2(d)-4.2(e). Similar features have been observed in prior numerical results [16, 46].

The crossflow Weber number of this simulation $W_e = 19$ falls into the bag breakup regime [6] where generally, due to a pressure differential, the center of the (spherical) droplet blows downstream while remaining attached to the rim. This pressure differential is caused by the high stagnation pressure on the front center of the drop and the low pressure in the separated wake region downstream [107, 108]. In the present simulations, similar behavior is observed although
Figure 4.2  Time history of $M_s = 1.47$ shock-column interaction and breakup with $We_a = 20$. The top half of each image depicts numerical Schlieren with liquid volume fraction shown in pink. The bottom half shows pressure contours with a $\phi_1 = 0.5$ iso-line at the gas-liquid interface.
Figure 4.3 Time history of $M_s = 2.5$ shock-column interaction and breakup with We$_a = 20$. The top half of each image depicts numerical Schlieren with liquid volume fraction shown in pink. The bottom half shows pressure contours with a $\phi_1 = 0.5$ iso-line at the gas-liquid interface.

The presence of the standing shock in the downstream recirculation region affects this pressure differential across the column such that the center does not push through.

Figure 4.3 depicts a time history of the We$_a = 20$ case with a shock Mach number of $M_s = 2.5$. Figure 4.3(a) depicts the time period shortly after the incident shockwave has impacted the water column with similar features observed to the lower Mach number simulation. However, the supersonic flow conditions cause the reflected shockwave to be significantly stronger and persists as a standing bow shock in front of the column, as observed in Figures 4.3(b)-4.3(d). As the water column begins to accelerate with the local flow, this bow shock gradually moves further upstream as the local relative velocity between the column and the air decreases.

The crossflow induced by the passage of the shockwave leads to continued deformation of the column in Figures 4.3(c)-4.3(f). In general, the pressure field and recirculation region downstream of the column appears to be considerably different from that of the lower Mach
number case. This is examined with comparisons at similar non-dimensional characteristic times between the $M_s = 1.47$ (left) and $M_s = 2.5$ (right) simulations in Figure 4.4. Streamlines are overlaid on the top half of each image. Note that while the acoustic Weber number is the same in each simulation, the crossflow Weber number is significantly different (estimated to be initially 19 and 245 for the $M_s = 1.47$ and $M_s = 2.40$ cases, respectively). As the presence of the standing shock in the $M_s = 1.47$ case appears to impact the bag formation, the shock structures observed in the $M_s = 2.5$ case affect the overall deformation behavior of the column. For example, a small standing shock appears just outside the water column surface in Figure 4.4(d) and locally affects the deformation of the column.

Finally, the length of the recirculation region in the $M_s = 1.47$ images depicted on the left side of Figure 4.4 grow over time. Interestingly, the recirculation length appears to correlate well with the length of the low pressure region measured from the liquid column to the downstream oblique shocks for the $M_s = 2.5$ simulation shown in the right column of Figure 4.4.

### 4.5.2 Effect of $\text{We}_a$

Figure 4.5 depicts a time history of the various $\text{We}_a$ cases with a shock Mach number of $M_s = 1.47$. The top half of each image depicts the numerical Schlieren or normalized exponentially spaced density gradient [131]. The bottom half depicts just the liquid volume fraction $\phi_1$ shown in blue. Each row of the figure corresponds to the same point in time with each column representing a different $\text{We}_a$. For this Mach number, the initial crossflow Weber number corresponds closely to the acoustic Weber number (see Table 4.2).

The observed breakup characteristics correlate well with the different regimes observed in experiments for Oh $< 0.1$. The regimes are listed in Table 4.3 where the transition Weber numbers are approximate partly due to the continuous nature of the breakup process and the arbitrary choice for specific transition points [6]. As a result, different researchers have reported slight variations on the transition between different regimes [68], however, the order in which they appear remains the same [110]. Figure 4.5(a) depicts the vibrational mode where the surface tension forces are large enough for the column to remain intact and oscillate as an ellipse.
Figure 4.4 Streamlines for the shock-column interaction with $\text{We}_s = 20$ for the $M_s = 1.47$ (left) and $M_s = 2.5$ (right) simulations. The top half of each image depicts streamlines overlaid on numerical Schlieren with liquid volume fraction shown in pink. The bottom half shows pressure contours with a $\phi_1 = 0.5$ iso-line at the gas-liquid interface.
Table 4.3 Breakup regimes and transition Weber number as given by [6].

<table>
<thead>
<tr>
<th>Regime</th>
<th>Weber Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vibrational</td>
<td>0 &lt; We &lt; ~11</td>
</tr>
<tr>
<td>Bag</td>
<td>~11 &lt; We &lt; ~35</td>
</tr>
<tr>
<td>Multimode</td>
<td>~35 &lt; We &lt; ~80</td>
</tr>
<tr>
<td>Sheet-thinning</td>
<td>~80 &lt; We &lt; ~350</td>
</tr>
<tr>
<td>Catastrophic</td>
<td>We &gt; ~350</td>
</tr>
</tbody>
</table>

Figures 4.5(b) and 4.5(c) depict various stages of the bag breakup regime which is observed to begin at a critical Weber number of We = 11 ± 2 [6]. Generally this regime is characterized by the growth of a bag structure where the center of the drop is blown downstream and attached to an outer rim. As previously mentioned, the presence of a standing shock downstream of the liquid column appears to affect the resulting bag structure in the present simulations.

The simulation in the multi-mode regime is depicted in Figure 4.5(d). In this regime, the center of the column is driven downstream more slowly leading to the creation of a bag/plume structure [132]. This behavior appears to be exaggerated by the presence of the standing shock previously mentioned with a substantial plume/bag-and-stamen structure forming. Finally, the numerical Schlieren depicts increasing amounts of liquid mass being stripped from the surface of the column as the Weber number increases into the lower end of the sheet-thinning regime in Figure 4.5(e).

Figure 4.6 depicts the history of the $M_s = 2.5$ simulations at various acoustic Weber numbers. Due to the higher flow speeds behind the shock, the estimated initial crossflow Weber number is much higher for each case compared to the corresponding $M_s = 1.47$ simulations (see Table 4.2).

Theofanous et al. [133] performed experiments of aerobreakup of spherical liquid droplets in $M = 3$ crossflows. They observed “piercing” ($44 < We < 10^3$) and “stripping” ($\sim 10^3 < We$) breakup regimes. The range of breakup features depicted in Figure 4.6 with the estimated effective Weber numbers varying from 46 in Figure 4.6(a) to 917 in Figure 4.6(e) appear to qualitatively match descriptions of those regimes despite the disparity in crossflow speeds ($M = 1.2$ for the $M_s = 2.5$ case versus $M = 3$ in the experiments) and flow dimensionality. In particular, a bag-and-stamen type structure is formed while at each timepoint (i.e. each row
Figure 4.5 Time history of $M_s = 1.47$ shock-column interaction. The number on the left side of each image row lists $t^* = t/t_c$, or the non-dimensional solution time scaled by the characteristic breakup time $t_c = \sqrt{\epsilon D/u}$ computed using post shock conditions. Each image shows liquid volume fraction in blue with the top half also showing numerical Schlieren.
of Figure 4.6), significantly more liquid mass can be observed stripping from the surface of the liquid column as the Weber number increases.

### 4.5.3 Drag coefficient and column trajectory

Finally, the drag coefficient and trajectory of the liquid columns is examined. Figure 4.7 depicts comparisons of the early stages of the drag coefficient with prior numerical results of Meng and Colonius [16], Chen [15], and Terashima and Tryggvason [46]. The drag coefficient was computed following [16]:

$$C_d = \frac{ma_c}{\frac{1}{2} \rho_g (u_g - u_c)^2 d_0}$$

where $d_0$ is the undeformed diameter of the column, $\rho_g$ and $u_g$ are the initial post-shock gas conditions and $u_c$ is the center of mass velocity given by equation 4.16. The acceleration is then computed using finite differences in time [16]:

$$a_c = \frac{d}{dt} \int \rho_1 \phi_1 udV.$$  

Good agreement is obtained with the data of [16], disparities in the other results can likely be attributed to the use of a different approach to calculate the drag coefficient, where drift data (and not averaged fluid velocity) is used to estimate the column acceleration. Refer to [16] and [129] for further discussion of different approaches for computing the drag coefficient.

Figure 4.8 depicts the drag coefficient at the later stages of the simulations with comparisons to an approximately rigid and stationary liquid column computed with a high liquid density ($\rho_l = 10,000$ kg/m$^3$) case with $We_a = 5$. This extra simulation was performed to provide a reference point to a stationary and rigid cylinder in crossflow where the drag coefficient is known. Generally for $100 < Re < 10^5$, the drag coefficient of a cylinder is known to be approximately 1 which agrees well with the present subsonic simulation with a crossflow Reynolds number of 1430. Meanwhile from Gowen and Perkins [134] the drag coefficient of a stationary cylinder in $M = 1.2$ flow is approximately 1.6. This agrees well with the minimum drag coefficient value computed for the simulation of the approximately rigid stationary cylinder which occurs around $t^* = 0.3$ in Figure 4.8. Variations of the drag coefficient in this simulation can be attributed to the gradual deformation of the high density column. Gowen and Perkins also noted there was
Figure 4.6 Time history of $M_s = 2.5$ shock-column interaction and breakup. The number on the left side of each image row lists $t^* = t/t_c$, or the non-dimensional solution time scaled by the characteristic breakup time $t_c = \sqrt{\epsilon D/u}$ computed using post shock conditions. Each image shows liquid volume fraction in blue with the top half also showing numerical Schlieren.
Figure 4.7 Drag coefficient comparison during the early stages for $M_s = 1.47$ (left) and $M_s = 2.5$ (right) compared to Meng and Colonius [16], Chen [15], and Terashima and Tryggvason [46].

Figure 4.8 Drag coefficient comparison at the later stages for $M_s = 1.47$ (left) and $M_s = 2.5$ (right) compared to Meng and Colonius [16].
almost no observed variation in the drag coefficient as a function of Reynolds number in the supersonic flow regime. Interestingly, the present results suggest for the liquid column there is significantly less variation in the drag coefficient as a function of the Weber number in the supersonic regime.

Overall, the drag coefficient exhibits significantly less unsteady variation compared to the results of [16], however, the general trend is similar. The differences can be attributed to the inclusion of surface tension, molecular viscosity, and interface sharpening employed in the current simulations. Lower drag coefficients are observed with lower Weber numbers for both shock Mach numbers. Significant differences in the drag as a function of the Weber number are observed in the $M_s = 1.47$ case in Figure 4.8(a). Consistent with the breakup behavior described previously, less variation is observed between the different Weber numbers in the $M_s = 2.5$ case as depicted in Figure 4.8(b).

Supporting the experimental observations of Temkin and Mehta [126], the unsteady drag is found to be larger in the decelerating relative flows of the liquid columns compared to that of the rigid stationary column. The coefficients are observed to be around twice as large as the rigid case for both shock Mach numbers at $We_a = 5$.

Figure 4.9(a) depicts the decreasing relative velocity of the liquid columns as a function of time with the velocity normalized by the post-shock gas velocity. The $M_s = 1.47$ case with $We_a = 5$ exhibited the lowest drag coefficient and correspondingly shows the highest
relative velocity at $t^* = 1.5$. Figure 4.9(b) shows the trajectories of the liquid mass over time. Interestingly, up to $t^* = 1.5$ the column trajectories largely collapse on each other when plotted against the characteristic time $t^*$.  

### 4.6 Conclusion

Numerical experiments of $M_s = 1.47$ and $M_s = 2.5$ shockwaves interacting with liquid columns are performed. The effects of compressibility, molecular viscosity, and surface tension are accounted for. The shockwaves induce a crossflow leading to aerobreakup of the liquid column. As the Weber number is varied several breakup modes are observed with good correlation to the experimentally observed breakup characteristics. The $M_s = 2.5$ shock leads to supersonic flow around the column. This affects the shape of the recirculation region behind the column and is observed to affect the corresponding deformation and breakup of the liquid. At higher Weber numbers there is an increase in the quantity of liquid mass stripped from the surface of the column. Lower Weber numbers resulted in lower observed drag coefficients for the liquid columns. However, depending on the Weber number the drag coefficients were still approximately two to three times those observed for a rigid liquid column.

### 4.7 Acknowledgments

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CHAPTER 5. CONCLUSIONS

The objective of this thesis is the numerical modeling of atomization in compressible flows. Atomization implies the presence of a discontinuous gas-liquid interface which can frequently undergo vast topological changes due to liquid breakup and merger. Across the discontinuity, the local curvature of the interface must be accurately computed in order to account for surface tension effects. This is further complicated by the possible interaction of the interface with shocks, expansion waves, and other complex flow features associated with high speed flows.

To address these challenges, a finite volume solver is developed. This began in Chapter 2 with development and validation of a code for solving the compressible multicomponent Euler equations using an HLLC Riemann solver for shock capturing and a PDE-based interface compression scheme to prevent numerical smearing of the material interface. Further development of these methods to incorporate the effects of capillary forces and the surface tension induced pressure jump across the gas-liquid interface was performed. With the resulting model, this jump is shown to be satisfied to within machine precision when the exact interface curvature is specified. A simple and efficient approach for numerically computing the interface curvature within the diffused interfaced region is also developed. As a result, no spurious deformation of the interface is observed in the simulation of a static droplet with surface tension (parasitic currents test), even without molecular diffusion terms included. The ability of the method is further demonstrated with simulations of an oscillatory elliptical droplet and a droplet-shock interaction problem.

The discretely non-conservative property of the interface compression scheme lead to the loss of under-resolved interfacial features during simulations. To address this, an alternative interface sharpening approach is examined and extended for use in the present model in Chapter 3. The approach, termed $\rho$-THINC based on its extension of the original THINC approach
to the phasic densities, is validated with various one and two-dimensional benchmark problems. It is then utilized to simulate primary and secondary atomization in compressible flows to demonstrate its robustness. Complex flow structures as well as liquid surface instabilities, breakup, and merger feature prominently in both two and three-dimensional simulations of a liquid jet in a $M = 2$ crossflow. The appearance of negative liquid pressures in the simulations suggests extensions of the model to account for liquid cavitation may be prudent in the future.

The effects of incident shock Mach number and surface tension on the secondary breakup of a cylindrical water column were investigated with a series of numerical experiments in Chapter 4. In particular, shock speeds of $M_s = 1.47$ and $M_s = 2.5$ were examined interacting with liquid columns of different diameters. Fluid immiscibility was maintained via the $\rho$-THINC interface sharpening procedure and the effects of compressibility, molecular diffusion, and surface tension are accounted for during the entire breakup process. The crossflow induced by the passage of the shockwave leads to aerobreakup of the liquid columns. In the subsonic case, the mode of breakup is strongly dependent on the Weber number and a number of regimes are captured with good correlation to the experimentally observed behavior. Higher Weber numbers demonstrate an increase in the amount of liquid mass stripped from the surface and higher average drag coefficients while lower Weber numbers lead to lower drag coefficients. In the supersonic case, less variation of the drag coefficient as a function of Weber number is observed. However, in all cases, the drag coefficient is observed to be significantly higher than that of an approximately rigid stationary column.

The solver developed in this thesis opens significant avenues for further research. While demonstration simulations of a liquid jet in supersonic crossflow were performed, detailed validation and parametric studies of physical parameters like the crossflow Mach number, momentum ratio, and Weber number are yet to be performed. In particular, quantifying their impact on the breakup and penetration properties of the jet would be useful. The computational complexity of three dimensional simulations is still relatively high, so further development of the code to utilize highly parallel SIMD (single instruction, multiple data) hardware such as graphics processing units (GPUs) or CPU-based coprocessors would be beneficial. Additionally, methods to relax the acoustic timestep restriction could expand the range of practical liquid
jet simulations that can be performed. The multiscale nature of atomization suggests adaptive mesh refinement (AMR) techniques would be useful as well. However, such improvements come at the cost of increased programming complexity. Various approaches for computing the interface curvature and normals also exist and can be investigated to compare their accuracy. The inclusion of additional physics such as cavitation, phase change, and thermal diffusion would extend the applicability of the model. Finally, it should be noted the five equation model employed is general for a number of different types of compressible interfacial flows and can be applied to problems which involve more than two components including gases, liquids, and even solids which utilize other equations of state such as van der Waals or Mie-Gruneisen [57].
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