TALBOT, JOSEPH WILLIAM. Numerical Studies of Aerated and Pure Liquid Jets in Supersonic and Subsonic Crossflows. (Under the direction of Dr. Jack Edwards.)

The requirements of scram and ramjet fuel injection systems to create adequate combustion conditions within very short residence times drives the need to better understand liquid jet into crossflow type problems. The effort documented herein contains the results of several numerical studies of such problems. Two primary cases are examined, an aerated-liquid jet into a supersonic crossflow and a pure-liquid jet into a subsonic crossflow. In these cases a variety of methods for better predicting and understanding these flow fields were explored, including Lagrangian particle tracking, sharp interface capturing schemes, and Eulerian droplet tagging. The supersonic case involves the incorporation of a one-way coupled Lagrangian particle method and a comparison of multiple Lagrangian droplet distributions. The subsonic case examines the difference in various implementations of sharp interface capturing schemes compared to a baseline piecewise parabolic reconstruction, as well as the examination of properties for unique liquid structures extracted directly from the Eulerian field data. The dependencies of the numerical solutions on time-step size and mesh resolution are also discussed. Results for all cases are compared to experimental data, primarily shadowgraph images and phase-Doppler particle analysis, for similar cases. The results throughout this project show good agreement with experimental data and the newly incorporated techniques have allowed for more in-depth analysis.
Numerical Studies of Aerated and Pure Liquid Jets in Supersonic and Subsonic Crossflows

by

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A thesis submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Master of Science

Aerospace Engineering

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DEDICATION

For my mother, who is the single most important factor for my academic success.
Joseph William Talbot was born in Carmel, New York a distant suburb of New York City to Deborah and Joseph P. Talbot. Talbot spent his life in this area until the completion of his primary education graduating from Carmel High School in 2011. After receiving his high school diploma, Talbot began the pursuit of his dream of becoming a test pilot by enrolling at Embry-Riddle Aeronautical University, seeking an undergraduate degree in Aerospace Engineering. Unfortunately, due to injuries sustained while a student at Embry-Riddle, Talbot’s goals were forced to shift towards work on the ground. Following the completion of his bachelor’s degree, Talbot fell into a role as a contractor working in software development, which he quickly decided was not for him. Talbot then left software for a better opportunity in numerical analysis for high-bypass turbofan engines. It was during his time in this position that Talbot decided to pursue further education, spurred by his newly found interest in numerical analysis and computational methods. Talbot approached Dr. Jack Edwards about the possibility of working as a member of his group at North Carolina State University and in August of 2017 Dr. Edwards offered Talbot a research assistantship. During his time at NCSU Talbot’s work primarily involved the use of numerical simulations to examine liquid jet into crossflow type problems. Talbot also pursued an internship with the Air Force Research Labs Directed Energy Directorate during this time, examining internal flows using numerical methods. In August of 2019 Talbot was offered and accepted a position as an Aeromechanical Engineer, returning to the world of turbine engine systems. In October of 2019 Talbot moved from North Carolina to Cincinnati, Ohio for this position during which time he completed the final stages of his degree at NCSU remotely. Talbot is expected to complete his Masters degree program at NCSU in December of 2019.
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INTRODUCTION

In the pursuit of sustained high Mach number flight, the gaze of the aerospace community has recently returned to the development of ram and scramjet propulsion systems. Ram and scramjet systems forgo the axial compressor of a turbojet, relying only on ram compression from the forebody and inlet surfaces of the craft. Although ram and scramjets are considered a modern emerging technology, the initial concepts date back over one-hundred years to the French scientist Rene Lorin in 1913. However, these initial concepts were cast aside after the conclusion that ram compression at low Mach numbers was insufficient to achieve adequate propulsive performance [1]. While these technologies didn't see much progression in the early days of aviation, they have now come to the forefront of research and development.

Following decades of slow growth in ram compression engines systems, the first flight of a ramjet occurred in 1949 when Languedoc Aircraft flew the Leduc 010. While this flight was a landmark in aerospace propulsion, the craft failed to reach supersonic speeds in any of its test flights. Over the next ten years the French company Nord Aviation developed the first turbo-ramjet combined cycle engine. This engine utilized the well-understood turbojet to power the aircraft until a speed at which it became efficient to transition to a ramjet mode of operation [1]. Through the rest of the 20th and early 21st centuries, aerospace groups around the world worked towards achieving stable prolonged ram and scramjet flight. Despite these efforts, the first successful flight test of a scramjet engine, by the Russian Central Institute of Aviation Motors (CIAM), did not occur until 1991. This vehicle was launched atop a specialized surface to air missile with incorporated flight test hardware. CIAM went on to use this test bed in cooperation with American and French efforts throughout the 1990s, achieving velocities greater than Mach 5 and altitudes over 85kft. Following these successful flights the NASA HYPER-X project, X-43, came into fruition. In June of 2001 a specially outfitted B-52 dropped the test aircraft over the Pacific. Once the craft was released, a Pegasus missile was used to achieve the required velocities for scramjet operation at which point the test bed separated from the missile. Two successful flight tests of the X-43 were conducted: one in which the vehicle achieved powered flight at Mach 7 and another which pushed operation to Mach 10 before demonstrating
its hypersonic glide capability [2]. A similar project followed after the X-43 - the X-51A. The X-51A was launched using a similar methodology to the X-43, the main differences in the flight of the two aircraft being the desired Mach number and fuel choice. While earlier efforts had used primarily highly energetic fuels such as hydrogen or ethylene, the X-51A moved toward using standard JP type hydrocarbon fuels. In May of 2010 the X-51A set a record for the longest scramjet burn of over 200 seconds while accelerating to Mach 5 [3]. Contemporary efforts are on-going by the governments of the United States, Russia, and China to further develop hypersonic flight vehicles primarily for defense purposes. Included in these efforts is the development of the Russian Zircon missile program which was reported to be capable of controlled hypersonic controlled flight as early as 2017. Recently this program was stated as being able to achieve speeds of Mach 9 with ranges over 1000 km [4].

In recent scram and ramjet engines such as those above it has become increasingly important to utilize computational fluid dynamics to improve on the design process and reduce some of the need for costly systems testing.

Throughout the progression of scramjet development the fuel of choice has shifted from highly energetic fuels to stable and widely used JP type fuels. While fuels such as hydrogen are easily vaporized and ignited (desirable properties for scramjet operation), they are also highly energetic and come with challenges in storage. These characteristics result in these highly reactive fuels failing to be insensitive munitions compliant, leading to safety and legal reasons for pursuing new options. As JP type fuels are both readily available and insensitive munitions compliant, they will likely become the primary fuel choice for scram and ramjet vehicles moving forward.

The switch from hydrogen and ethylene based fuels to hydrocarbon fuels in scramjets is not without challenges. Under cruise conditions, residence times for air traveling from the inlet to the nozzle of the engine are on the order of milliseconds. While formerly the challenge of igniting and sustaining combustion within a scramjet was met by using large injectors spouting highly vaporized and reactive fuel, new methods will need to be developed in order to meet these challenges using hydrocarbon based fuels. In injecting liquid fuels three primary areas of concern exist; ensuring proper fuel air mixing, ensuring sufficient residence times, and ensuring sufficient fuel mass flow rates into the engine. The last of these three issues can largely be solved by simply adding additional injectors along the interior of the engine, effectively multiplying the total fuel mass flowing into the system. Increasing residence times has been the subject of many efforts, especially concerning the interior geometry of the engine using ramps and backward facing steps to entrain flow for long enough times to achieve and sustain adequate combustion. The mixing problem has so far proved to be challenging. Several studies have been performed into the mixing conditions created by various types of injectors situated in various locations of the flow. One such option is to inject a gas upstream of the injector exit to create a fuel air mixture and encourage primary breakup before the fuel reaches the combustor. These injectors are known as barbotage or aerated-liquid fuel injectors. In studies such as those by Lin et al. [5] [6] these aerated-liquid injectors are examined for fuel injection under various liquid-gas mixture ratios into subsonic and supersonic crossflows. A portion of the examination of these various injectors is dedicated to observing how a pure liquid jet
(without aerating gas) deforms and breaks up as it encounters a crossflow. These breakup modes are of critical importance in creating an suitable environment for combustion through the atomization of the spray.

The examination of injectors for scramjet applications have been the subject of much effort from various organizations including the Air Force Research Lab. For this work the experiments performed at AFRL’s Wright-Patterson facility [5] are specifically considered. In this study, an aerated-liquid jet was injected into a Mach 1.94 crossflow for two gas-liquid ratios (GLR). Using shadowgraph imaging and phase Doppler particle analysis, the temporal evolution of jet structures in the crossflow were examined. The study examined the effects of several parameters such as nozzle type, gas-liquid ratios, and injector height on the plume penetration and breakup. The study showed that the liquid jet viewed in a cross-stream plane is largely contained within a kidney like shape, with larger droplets about its periphery. From the shadowgraph images created in this study, the breakup of the liquid jet can be observed. The breakup process shown involves the development and break off of a relatively large protrusion of liquid from near to the top of the primary jet as it begins to turn with the crossflow.

Additional experiments have also been performed for pure liquid jets into subsonic crossflows by Sallam et al. [7]. In these experiments the effects of increasing Weber numbers were examined by shadowgraph and holograph imaging techniques. This study demonstrated that changes in crossflow Weber number induce different breakup modes. This study observed that for high Weber numbers (We > 110) the jet enters a shear breakup regime. In this regime, it is noted that instabilities form on the upwind surface of the liquid jet as a result of acceleration of a fluid of lesser density pushing against a fluid of greater density. This is called a Rayleigh-Taylor instability. These instabilities are then seen to form ligaments along the outside of the jet which then separate from it. As these ligaments stretch, they eventually terminate as individual droplets break away from their ends. As the main body of the jet continues into the crossflow, the instabilities grow in size, resulting in larger bodies breaking away. This continual breakup eventually results in the destruction of any observable main liquid jet in the far downstream region.

Using the above experimental data as a resource for validation, efforts have been made to further the state of NCSU’s REACTMB multiphase solver’s capabilities. Successful modeling and validation of the breakup process for liquid fuel injection would allow further numerical studies to examine critical parameters with regard to promoting combustion within a scramjet engine. From these sets of experiments two studies were chosen for analysis throughout this work. The first is the study of an aerated-liquid jet in a supersonic crossflow, corresponding to the work of Lin et al. [5]. The second involves the study of a pure-liquid jet in a subsonic crossflow for a fixed Weber number, corresponding to the work of Sallam et al. [7]. Both studies utilize the same underlying framework of REACTMB, however each of the two examines the use of different additional methods of simulation or analysis. The aerated-liquid in a supersonic crossflow study focuses specifically on the use of Lagrangian droplet tracking methods for the examination of spray distribution and breakup. Two areas are the subject of investigation in the pure-liquid jet into subsonic crossflow study: the use of sharp interface capturing schemes and the incorporation of an Eulerian droplet
tagging methodology to extract spray statistics. Various sharp interface capturing schemes are evaluated for their ability to capture the fine liquid structures generated by the breakup process. Brief comparisons are also made between two mesh resolutions in both studies.

Both studies in this work utilize numerical simulation to examine time accurate two-phase flow mixing and breakup for a liquid jet in crossflow. All of the work herein utilizes a volume of fluid (VOF) method for the capture of interfaces within the multiphase flow. The volume of fluid method originally published by Hirt and Nichols in 1981 is based on earlier marker-and-cell type methods [8]. The volume of fluid method advects a function that describes whether a particular cell contains a liquid, gas, or lies on the interface of the two. Improvements have since been made to this method using geometric reconstructions after the advection of this function, including the simple line interface calculation (SLIC) [9] and the piece-wise linear interface calculation (PLIC) [10][11][12][13][14]. While the PLIC method in particular provided significant improvement, it is accompanied by major drawbacks in the form of implementation complexity in three-dimensional cases as well as heavy computational costs. As such efforts have been made to improve volume of fluid methods by reducing computational costs while maintaining accuracy. One such method is the Tangent Hyperbolic INterface Capturing (THINC) method, originally developed by Xiao et al. [15]. The THINC method avoids the expensive geometric reconstruction by use of a hyperbolic tangent function as the basis for intercell discontinuity reconstruction.

Earlier work has been performed in applying THINC specifically to fuel injection problems [16]; however, most of this work has been concerned primarily with flow inside injectors. Efforts to further the earlier work for liquid jet in crossflow problems have been presented in [17],[18],[19], in which various methods of imposing injector conditions into a crossflow were explored. These studies examined the breakup of liquid jets in quiescent air as well as subsonic and supersonic crossflows.

Another scheme utilized for improving the capturing of interfaces in a two-phase flow is the Boundary Variation Diminishing scheme (BVD). The BVD scheme was originally developed by Sun et al [20] and aims to reduce the magnitude of discontinuities at cell boundaries. In order to accomplish this, BVD schemes dynamically switch between sharp (THINC) and smooth (PPM) reconstructions in a particular cell, based on which reconstruction minimizes diffusive error at a cell interface. Several implementations of this method are discussed by Deng et al. in [21].

In addition to the examination of sharp interface capturing schemes, the pure-liquid in subsonic crossflow study also examines the use of a droplet tagging method for the extraction of Eulerian solution information regarding each unique liquid structure in a given domain. This method, based on the work of Herrmann [22], can be used to collect statistics for unique liquid structures present in a given simulation. Efforts have also been made to incorporate the Lagrangian particle tracking method developed in [23] for assumed initial droplet distributions in [24] as well as methods to incorporate the breakup of these droplets [19]. The aerated-liquid jet into supersonic crossflow study focuses primarily on the results gathered from the implementation of this Lagrangian particle tracking method. It is expected that in future work, the Eulerian droplet tagging information will be

4
used to seed Lagrangian particles during solver run time.

This document outlines the results of both of these studies starting from the governing equations and numerical methods used within the REACTMB solver. These sections elaborate on both the methods being evaluated in these studies as well as the underlying methods used by the solver. Following this a discussion of the experimental and computational setups for both studies is given. Then, results for the aerated-liquid jet in supersonic crossflow are shown including the use of the Lagrangian particle tracking method. The results concerning the pure-liquid jet in a subsonic crossflow are then examined, including both the results of different sharp interface capturing schemes and an examination of the data extracted using Eulerian droplet tagging methods. Finally, a brief conclusion is given with respect to the works as a whole which includes the discussion of potential areas for future efforts.
CHAPTER 2

GOVERNING EQUATIONS

The flow solver used throughout this work, REACTMB-MP employs the isothermal Navier-Stokes equations for a two-phase mixture as outlined below:

$$\Omega \frac{\partial \vec{U}}{\partial t} + \sum_k (\vec{E} - \vec{E}_v) \cdot \vec{n}_k A_k - \Omega \vec{S} = 0$$ (2.1)

where $\Omega$ is the volume of the cell, $A_k$ is the face area, and $\vec{n}_n$ is the outward normal vector, and $\vec{S}$ is a vector of source terms. The inviscid flux vector $\vec{E} \cdot \vec{n}_k$ is as follows:

$$\vec{E}_k \cdot \vec{n}_k = \vec{u}_k \begin{bmatrix} \rho v \alpha \\ \rho \\ \rho u \\ \rho v \\ \rho w \end{bmatrix}_k + \begin{bmatrix} 0 \\ 0 \\ n_x \\ n_y \\ n_z \end{bmatrix}_k p_k$$ (2.2)

where $u$, $v$, and $w$ are components of the velocity vector, $p$ is the pressure, and $\rho$ is the mixture density. The conservative and primitive variables for this formulation are defined as $\vec{U}$ and $\vec{V}$ respectively.

$$\vec{U} = \begin{bmatrix} \rho v \alpha \\ \rho \\ \rho u \\ \rho v \\ \rho w \end{bmatrix}, \quad \vec{V} = \begin{bmatrix} \alpha \\ p \\ u \\ v \\ w \end{bmatrix}$$ (2.3)

The mixture density is defined as

$$\rho = \rho_v \alpha + \rho_l (1 - \alpha)$$ (2.4)
where $\alpha$ is the vapor phase volume fraction defined as follows:

$$
\alpha = \begin{cases} 
0 & \text{if completely liquid} \\
0 < \alpha < 1 & \text{if within an interface} \\
1 & \text{if completely vapor}
\end{cases}
$$

The ideal gas law is used to define the vapor-phase density as follows:

$$
\rho_v(P) = \frac{P}{RT}
$$

The liquid density and viscosity are set to 993.5 kg/m$^3$ and 8.93x10$^{-4}$ kg/(m-s), respectively. Viscous fluxes are implemented for a Newtonian fluid as shown below for the i-direction:

$$
E_{v,i} = \begin{bmatrix} 
-\rho Y_l Y_v u_{r,i} \\
0 \\
t_{xx} \\
t_{yx} \\
t_{zx}
\end{bmatrix}
$$

where $t_{ij}$ is defined as follows:

$$
t_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{i,j} \frac{\partial u_k}{\partial x_k} \right)
$$

Equation (2.9) is used as a closure for the system

$$
\mu = \mu_v \alpha + \mu_l (1 - \alpha)
$$

The source vector $\vec{S}$ is defined as

$$
\vec{S} = \begin{bmatrix} 
0 \\
0 \\
F_{sv,x} \\
F_{sv,y} \\
F_{sv,z}
\end{bmatrix}
$$

where $F_{sv}$ are the surface forces defined below

$$
F_{sv} = \sigma \kappa \delta_s \vec{n}
$$

in which $\sigma$ is water-air constant surface tension of 0.072 N/m, $\kappa$ is the curvature of the surface, and $\delta_s$ is a delta function on the surface. A continuum surface force (CSF) model is used to calculate these surface forces. The CSF model, originally developed by Brackbill et al., "interprets surface tension as a continuous, three-dimensional effect across an interface, rather than as a boundary
value condition on the interface. [25]”. This model was then further improved by Lafaurie et al. who equates surface tension to the divergence of the capillary pressure tensor \( T \) the derivation of which can be seen in [26]. The resulting equation is as follows:

\[
T_{i,j} = -\sigma (\delta_{i,j} - \tilde{n}_i \tilde{n}_j) \delta_s
\]  

(2.12)

where

\[
\sigma k n \delta_s = -\nabla \cdot T
\]  

(2.13)

\( \delta_s \) is defined as a delta function on the surface such that

\[
\delta_s = \delta(\zeta_3)
\]  

(2.14)

\( \zeta_3 \) is a component of a system of orthogonal, normalized, curvilinear coordinates \( (\zeta_1, \zeta_2, \zeta_3) \) defined such that the surface is the locus of the points where

\[
\zeta_3 = 0
\]  

(2.15)

A smoothed color function for the volume fraction is then used blend values between 0 and 1 over the finite interface. A smoothed color function is used in order to avoid computing the gradients of a steep function that would result in a non-physically skewed surface tension. This color function is defined as follows:

\[
\tilde{a}(x) = \int_v \alpha(x') H(x - x'; \epsilon) d x'
\]  

(2.16)

where \( H \) is a smoothed integral function. The color function is then implemented using a two delta filtering method. This method considers a three node stencil in each dimension over which a weighted box average is first computed for each octant. Then a second weighted box average is taken using the octant average values. This can be expressed in the discrete form below:

\[
\tilde{a} = \Sigma w_k \alpha
\]  

(2.17)

where \( w_k \) are weights chose to approximate the two delta box filtering method. Coordinate indices are defined for each neighboring cell \( k \) as \( i + a_k, j + b_k, k + c_k \), where \( a_k, b_k, \) and \( c_k \) can have values of -1, 0, or 1. Following this definition the weights, \( w_k \), can be expressed as follows

\[
w_k = (1/2)^3 - |a_k| + |b_k| + |c_k|
\]  

(2.18)

From the above equations (2.12), (2.13), and (2.16) we are able to redefine the surface tension forces, \( F_{sv} \), as follows:

\[
F_{sv,i} = \int_A \sigma (\delta_{i,j} - \tilde{n}_i \tilde{n}_j) n_j dA
\]  

(2.19)
where $\vec{n}_i$ is the phase interface normal vector defined as

$$\vec{n}_i = \frac{\nabla \tilde{a}}{|
abla \tilde{a}|}$$  \hspace{1cm} (2.20)

Further discussion of the implementation for surface tension can be found in [16].
Within this chapter numerical techniques and considerations for the implementation of an all-speed two-phase flow solver for use in liquid jet in crossflow simulations are discussed.

### 3.1 Flux Splitting

REACTMB-MP utilizes the Low Diffusion Flux Splitting Scheme (LDFSS) an extension of the Advection Upstream Splitting Method (AUSM)\(^1\) originally created by Edwards in 1997\(^2\) and further extended to real fluids in \(^3\),\(^4\). The implementation of this scheme for multiphase flows that was followed in this work is outlined in Cassidy et. al\(^5\). This specific scheme, LDFSS-2001, maintains pressure-velocity coupling at low speeds while exactly capturing a stationary contact wave aligned with a grid boundary. Mechanisms are also incorporated for pressure and velocity diffusion in order to suppress oscillations at low speeds. In this scheme, interface flux terms are split into convective and pressure contributions as follows:

\[
\vec{E}_{i+1/2} \cdot \vec{n}_{i+1/2} = [\vec{E}_{c,j+1/2}(\vec{V}_{L,i+1/2}, \vec{V}_{R,i+1/2}) + \vec{E}_{p,j+1/2}(\vec{V}_{L,i+1/2}, \vec{V}_{R,i+1/2})] \cdot n_{i+1/2} \tag{3.1}
\]

where the convective terms are

\[
\vec{E}_{c,i+1/2} \cdot \vec{n} = U_{i+1/2}^+ \begin{bmatrix} \rho v \\ \rho \\ \rho u \\ \rho v \\ \rho w \end{bmatrix}_L + U_{i+1/2}^- \begin{bmatrix} \rho v \\ \rho \\ \rho u \\ \rho v \\ \rho w \end{bmatrix}_R \tag{3.2}
\]
in which \( L \) and \( R \) denote left and right states respectively. Split velocity components are then defined as

\[
U_{i+1/2}^+ = \tilde{a}_{c,1/2} \left[ M_L^+ - M_{1/2} \left(1 - \frac{P_L - P_R + |P_L + P_R|}{2\rho_L V_{ref,c,1/2}^2} \right) \right]
\] (3.3)

\[
U_{i+1/2}^- = \tilde{a}_{c,1/2} \left[ M_R^- - M_{1/2} \left(1 - \frac{P_L - P_R + |P_L + P_R|}{2\rho_R V_{ref,c,1/2}^2} \right) \right]
\] (3.4)

In order to define the above split Mach number within this work, a harmonic weighted mean sound speed for a two-fluid system (originally derived by Wallis [32]) is used as defined below:

\[
\frac{1}{a^2} = \frac{1}{\rho_v a_v} + \frac{1}{\rho_l a_l} \left( \frac{\rho_l a_v}{a_v^2} + \frac{\rho_v a_l}{a_l^2} \right)
\] (3.5)

where

\[ a_v = \sqrt{RT_{\infty}}, \quad a_l = 1500 \text{m/s} \] (3.6)

The following equations are then used to describe the split Mach number

\[ a_{L/R} = \frac{1}{2} \left(1 \pm \text{sign}(1, M_{L/R})\right) \] (3.7)

\[ \beta_{L/R} = -\max(0, 1 - \text{int}(|M_{L/R}|)) \] (3.8)

\[ M_{L/R}^\pm = a_{L/R}(1 + \beta_{L/R})M_{L/R} \pm \frac{1}{4} \beta_{L/R}(M_{L/R} \pm 1)^2 \] (3.9)

where

\[ M_{L/R} = \frac{\hat{u}_{L/R}}{a_{1/2}} \] (3.10)

in which \( \hat{u} \) is the face normal velocity component.

\[
\hat{u}_{L/R} = n_{x,i+1/2} u_{L/R} + n_{y,i+1/2} v_{L/R} + n_{z,i+1/2} w_{L/R}
\] (3.11)

This results finally in the below Mach number definition.

\[
M_{1/2} = \frac{1}{2} \left[ M_L^+ - \frac{1}{2}(M_L + |M_L|) - M_R^- + \frac{1}{2}(M_R - |M_R|) \right]
\] (3.12)

Throughout the above, the one-half terms are arithmetic averages as defined below except in the case of the sound speed and Mach number.

\[ [\cdot]_{1/2} = \frac{1}{2}([\cdot]_L + [\cdot]_R) \] (3.13)
Turning attention to the pressure contributions to the flux we further describe them as

\[ \vec{E}_{P,i+1/2} \cdot \vec{n}_{i+1/2} = \begin{cases} 0 \\ 0 \\ n_x \\ n_y \\ n_z \end{cases} \cdot P_{i/2} \] (3.14)

The below pressure splitting is then used to calculate \( P_{i/2} \)

\[ D_{L/R}^\pm = \alpha_{L/R}(1 + \beta_{L/R}) - \frac{1}{2} \beta_{L/R}(1 \pm M_{L/R}) \] (3.15)

\[ P_{i/2} = \frac{1}{2} \left[ P_L + P_R + \frac{1}{2}(D_L^+ - D_R^-)(P_L - P_R) + \rho_{i/2} V_{ref,1/2}^2(D_L^+ + D_R^- - 1) \right] \] (3.16)

where

\[ V_{ref,1/2}^2 = \min(a_1^2/2, \max((\vec{u} \cdot \vec{u})_{1/2}, U_{ref}^2)) \] (3.17)

A higher order extension to LDFSS was later made utilizing the piecewise parabolic method (PPM) developed by Colella and Woodward [33]. The use of this PPM scheme requires a seven point stencil in each direction. Given the set of primitive variables as listed in Equation (2.3), left and right state values \( \vec{v}_{L,R,i+1/2} \) are defined by the following set of equations:

\[ \Delta \vec{v}_i = \vec{v}_{i+1} - \vec{v}_i \] (3.18)

\[ S_i = \frac{1}{2}(\Delta \vec{v}_i + \vec{v}_{i-1}) \] (3.19)

\[ \vec{v}_{L,i+1/2} = \vec{v}_{R,i+1/2} = \frac{1}{2}(\vec{v}_i + \vec{v}_{i+1}) + \frac{1}{6}(S_i + S_{i+1}) \] (3.20)
To ensure monotonicity the following algorithm is then utilized:

\[
\text{if sign}[(\vec{V}_{L,i+1/2} - \vec{V}_i)(\vec{V}_i - \vec{V}_{R,i-1/2})] = -1, \text{then} \\
\vec{V}_{L,i+1/2} = \vec{V}_{R,i-1/2} = \vec{V}_i \\
\text{else} \\
C = \vec{V}_{L,i+1/2} - \vec{V}_{R,i-1/2} \\
D = 6[\vec{V}_i - \frac{1}{2}(\vec{V}_{L,i+1/2} + \vec{V}_{R,i-1/2})] \\
\text{if}(D > C), \text{then} \\
\vec{V}_{R,i-1/2} = 3\vec{V}_{i} - 2\vec{V}_{R,i-1/2} \\
\text{else if}(-C > D), \text{then} \\
\vec{V}_{L,i+1/2} = 3\vec{V}_{i} - 2\vec{V}_{R,i-1/2} \\
\text{end if} \\
\text{end if}
\] (3.21)

3.2 Time Advancement and Preconditioning

Preconditioning allows for compressible flow codes to operate efficiently and accurately at low Mach numbers. In order to accomplish this for the code used herein, a form of Chorin’s artificial compressibility method is used [34]. The governing equations of Chapter 2 are affected by preconditioning as follows:

\[
\Omega P \frac{\partial \vec{V}}{\partial \tau} + \Omega \frac{\partial \vec{U}}{\partial t} + \sum_k (\vec{E} - \vec{E}_v)_k \cdot \vec{n}_k A_k - \Omega \vec{S} = 0
\] (3.22)

where \(\tau\) is an artificial sub-iteration time-step and \(P\) is the preconditioning matrix defined as follows:

\[
P = \begin{bmatrix}
\rho & \frac{\partial \rho v}{\partial p} + \Theta \frac{\rho a}{\rho} & 0 & 0 & 0 \\
\rho v - \rho_l & \frac{\partial \rho}{\partial p} + \Theta & 0 & 0 & 0 \\
u(\rho v - \rho_l) & \frac{\partial \rho}{\partial p} + \Theta u & \rho & 0 & 0 \\
v(\rho v - \rho_l) & \frac{\partial \rho}{\partial p} + \Theta v & 0 & \rho & 0 \\
\rho w(\rho v - \rho_l) & \frac{\partial \rho}{\partial p} + \Theta w & 0 & 0 & \rho
\end{bmatrix}
\] (3.23)

where \(\vec{v} = \frac{\partial p}{\partial \vec{V}} = [0, 1, 0, 0, 0]^T\), \(\Theta = \left(\frac{1}{V_{r e f}^2} - \frac{1}{a^2}\right)\), and \(V_{r e f}\) is defined as it is in the above section. For flows such as those being considered in this document, a transition to supersonic flow is possible.
Eigenvalues of the above preconditioned equation system appear as follows:

\[ \lambda_1 = \bar{u} \cdot \bar{n} \]

\[ \lambda_{2,3} = (1 + M_{\text{ref}}^2) \bar{u} \cdot \bar{n} + \sqrt{(1 - M_{\text{ref}}^2)^2(\bar{u} \cdot \bar{n})^2 + 4V_{\text{ref}}^2} \]

\[ \frac{1}{a^2} = \frac{1}{\rho_v a_v + \rho_l a_l} \left( \rho_v a_v + \rho_l a_l \right), a_v = \sqrt{RT} \infty, a_l = 1500 \text{ m/s} \]  

(3.24)

\[ V_{\text{ref}}^2 = \min(a^2, \max(\bar{u} \cdot \bar{u}, U_{\text{ref}}^2)) \]

\[ M_{\text{ref}}^2 = \frac{V_{\text{ref}}^2}{a^2} \]

where \( a \) is the harmonic weighted two-phase sound speed, \( a_v \) is the vapor phase sound speed, and \( a_l \) is the liquid phase sound speed. The reference velocity \( V_{\text{ref}} \) has been noted to have significant impact on the solution and its convergence. Examinations of different variations of the term can be found in [31] and [35]. The reference Mach number \( M_{\text{ref}} \) is defined as a function of reference velocity and the previously mentioned Mach number. The reference velocity \( U_{\text{ref}} \) is generally defined as the maximum expected velocity. In the subsonic cases discussed herein this value is defined as \( U_{\text{ref}} = 100 \text{ m/s} \). In the supersonic cases preconditioning is not used and \( V_{\text{ref}} = a^2 \) is used. Derivations of these eigenvalues can be found in Appendix A.

A dual-stepping time advancement method is utilized throughout this work. The specific methodology used is as presented in [31]. At each sub-iteration \( k \), the following system is solved.

\[
\begin{align*}
\Omega \left( \frac{1}{\Delta t} P + \frac{3}{2\Delta t} \frac{\partial \bar{U}}{\partial \bar{V}} \right) + \frac{\partial \bar{R}}{\partial \bar{V}} & \approx \Delta \bar{V}^{n+1,k} \\
- \left[ \frac{\Omega}{\Delta t} \left( \frac{3}{2} U^{n+1,k} - 2U^n + \frac{1}{2} U^{n-1} \right) + \left( \sum_k (\bar{E} - \bar{E}_v)_k \cdot \bar{n}_k A_k - \Omega^3 \right) \right]
\end{align*}
\]

(3.25)

The solution is then updated as follows:

\[ \bar{V}^{n+1,k+1} = \bar{V}^{n+1,k} + \Delta \bar{V}^{n+1,k} \]

(3.26)

In order to solve the above system, an incomplete LU matrix decomposition is employed. A Jacobian is constructed from local Jacobians of fluxes, seen above as \( \frac{\partial }{\partial \bar{V}} \bar{R} \). However, a loss of diagonal dominance in cases of large changes over a fluid interface is asserted by Pan [36], which may make the incomplete LU system much less robust. In order to prevent this issue, the below linearization of the system is used:

\[
\frac{\partial \left( \bar{E}_{i+1/2} \cdot \bar{n}_{i+1/2} - \bar{E}_{i-1/2} \cdot \bar{n}_{i-1/2} \right)}{\partial \bar{V}} \Delta \bar{V} \approx A_{i+1/2}^+ \Delta \bar{V}_{i+1} + \frac{1}{2} \left[ (A_{i+1/2}^+ - A_{i-1/2}^+) + (A_{i+1/2}^- - A_{i-1/2}^- - 1/2) \right] \Delta \bar{V}_i - A_{i-1/2}^- \Delta \bar{V}_{i-1}
\]

(3.27)

Small times steps are still required due to the need to resolve fine-scale flow features. In the cases
discussed throughout this work, time-steps are of the range of $5.0 \times 10^{-7}$ to $1.0 \times 10^{-6}$. These small time-steps are primarily due to rapidly moving phase interfaces during liquid jet injection.

### 3.3 Sharp Interface Capturing

Sharp interface capturing techniques are used in this work to enhance the resolution of liquid-vapor interfacial behavior. Three such techniques are explored throughout this work, two variations of a tangent hyperbola interface capturing (THINC) scheme and one boundary variation diminishing (BVD) scheme.

#### 3.3.1 THINC

THINC, originally developed by Xiao et al [15], employs a hyperbolic tangent function to model the variation of the volume fraction within a cell in place of the polynomial description used by PPM or TVD methods. Two implementations of THINC schemes are used in this work. The first is the THINC Exact Monotone (THINC-EM), originally described in [37] and later improved upon in [31], which is dependent on the local CFL number. The second implementation is based on the method described by Shyue et al. in [37]. This method removes the local CFL dependence from the system and normalizes the reconstruction to always lie between zero and one.

#### 3.3.1.1 THINC-EM (Case A)

The THINC-EM scheme allows the connection of any two states of any generic variable, in our case volume fraction. These two states are monotonically connected by the following generic form of the method:

$$\alpha_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} a(x) \, dx$$  \hspace{1cm} (3.28)

where $a(x)$ is defined as:

$$\alpha_i = \frac{a_{max}}{2} \left[ 1 + \tanh(\beta \left( \frac{x - x_{i-1/2}}{x_{i+1/2} - x_{i-1/2}} - \tilde{x}_i \right) \right]$$  \hspace{1cm} (3.29)
$\beta$ above is a sharpening factor unless otherwise noted this value was held at a constant of 3.5 throughout this work. The algorithm used to reconstruct this volume fraction are as follows:

$$a_{L,i+1/2} = a_{min} + \frac{1}{2}(\alpha_{max} - \alpha_{min})(1 - SG^+)$$

$$a_{R,i-1/2} = a_{min} + \frac{1}{2}(\alpha_{max} - \alpha_{min})(1 - SG^-)$$

$$G^+ = \frac{1}{\beta C_{i+1/2}} \log[\cosh(\beta C_{i+1/2} - \sinh(\beta C_{i+1/2}B^+))]$$

$$G^- = \frac{1}{\beta C_{i-1/2}} \log[\cosh(\beta C_{i-1/2} - \sinh(\beta C_{i-1/2}B^-))]$$

$$B^+ = \frac{1}{\tanh(\beta)} \left(1 + \frac{\cosh(\beta)}{T^+}(\tanh^2(\beta) - 1]\right)$$

$$B^- = \frac{1}{\tanh(\beta)} \left(-\frac{T^-}{\cosh(\beta) - 1}\right)$$

$$T^+ = \exp \left[\beta S \left(\frac{2(a_{L,i+1/2} - \alpha_{min} + \epsilon)}{\alpha_{max} - \alpha_{min} + \epsilon} - 1\right)\right]$$

$$T^- = \exp \left[\beta S \left(\frac{2(a_{R,i-1/2} - \alpha_{min} + \epsilon)}{\alpha_{max} - \alpha_{min} + \epsilon} - 1\right)\right]$$

where the index 'i' corresponds to a given cell and the indexes 'i+1/2' and 'i-1/2' represent the faces bounding that cell. The terms listed below are used to bound the reconstructed volume fractions at cell interfaces to lie between the volume fractions at $a_{R,i+1/2}$ and $a_{L,i-1/2}$

$$a_{min} = \min(a_{i+1}, a_{i-1})$$

$$a_{max} = \max(a_{i+1}, a_{i-1})$$

$$S = \text{sign}(a_{i+1} - a_{i-1})$$

Within this implementation, initial monotone reconstruction of the volume fraction is needed as a basis for the sharpening strategy. The initial reconstruction used for this purpose is that shown above in Equation (3.31). The response of this scheme is directly affected by the rate at which the interface propagates across the cell. A local CFL number is defined to control this rate.

$$C_{i+1/2} = \min(1, \max(-1, \frac{\tilde{n}_{i+1/2} \cdot \tilde{n}_{i+1/2} \Delta t}{\Delta x_{i+1/2} \cdot \tilde{n}_{i+1/2}}))$$

$$C_{i+1/2}^+ = \max(\epsilon, C_{i+1/2})$$

$$C_{i-1/2}^- = \min(\epsilon, C_{i+1/2})$$

where $\epsilon$ is a small number used to prevent division by zero errors. In cases where the local CFL exceeds one, the model sets the left or right state for the volume fraction to local cell-interface values as determined by the initial reconstruction. The performance of this scheme is directly dependent on the above defined interface CFL. The best interface capturing performance occurs when the
local CFL is small or is set to zero. The choice to not simply and directly set this value to zero comes following earlier work mentioned in [16] where non-physical transfers of mass across interfaces as well as pockets of unresolved fluid were observed.

### 3.3.1.2 Time-Step Independent (Case B)

The second implementation of a THINC scheme is based on the method that was derived by Shyue [37] and is the case in which the limit of the above mentioned local CFL number approaches zero. This formulation normalizes the reconstructed variable to lie between zero and one and is based on the following hyperbolic tangent function which differs slightly compared to that in the previous scheme:

\[
\Phi_i(x) = \frac{1}{2} \left[ 1 + \tanh(\beta (\frac{x - x_i - 1/2}{\Delta X_i} - \bar{x}_i)) \right]
\]

(3.33)

The implementation of this case is outlined as follows:

\[
L = \exp(S\beta(2.0 \alpha_{L,i+1/2} - \alpha_{min} + \epsilon))
\]

\[
T = \frac{1}{\tanh(\beta)} \left( \frac{L}{\cosh(\beta)} - 1 \right)
\]

\[
\alpha_{L,i+1/2} = \alpha_{min} + \frac{1}{2}(\alpha_{max} - \alpha_{min})(1 + S\tanh(\beta + T))
\]

\[
\alpha_{R,i-1/2} = \alpha_{min} + \frac{1}{2}(\alpha_{max} - \alpha_{min})(1 + ST)
\]

where the same limiting terms apply from the THINC-EM method discussed above. A one-dimensional comparison of the resulting interface values for these first two schemes at varying CFL conditions can be seen in Appendix B.

### 3.3.2 BVD (Case D)

One additional approach was used for improving the capturing of phase interfaces in this work. This method, is known as a Boundary Variation Diminishing (BVD) scheme and was originally put forth by Sun et al. [20], seeks to reduce the diffusive error at the cell interfaces by minimizing the jump in reconstructed variables. The BVD method allows for switching between a polynomial reconstruction and a sharp reconstruction that allows for discontinuities to exist partly within a cell instead of entirely at the cell interface. The implementation used for this method is described as BVD Algorithm #4 of [21]. The first step in this method is to compute the total boundary variation (TBV) of the target cell for each of the PPM and THINC solutions, defined as TBV\textsuperscript{T} and TBV\textsuperscript{P} respectively.

\[
TBV^T = |\alpha_{L,i-1/2}^{T} - \alpha_{R,i-1/2}^{T}| + |\alpha_{L,i+1/2}^{T} - \alpha_{R,i+1/2}^{T}|
\]

\[
TBV^P = |\alpha_{L,i-1/2}^{P} - \alpha_{R,i-1/2}^{P}| + |\alpha_{L,i+1/2}^{P} - \alpha_{R,i+1/2}^{P}|
\]

(3.35)
Then a comparison is made in order to choose the reconstruction used for the cell.

\[
\alpha_i(x) = \begin{cases} 
\alpha^T_i & \text{if } \text{TBV}_i^T < \text{TBV}_i^P \\
\alpha^P_i & \text{otherwise}
\end{cases}
\]  

(3.36)

Left and right state values are then computed using the values from the chosen reconstruction.

### 3.4 Lagrangian Droplet Tracking

A droplet tracking engine is utilized for portions of this work. The method used was originally implemented within REACTMB in Kulkarni and Edwards [23] and further improved upon in [38]. The framework developed within this package includes the ability to find the location of droplets in a multi-block mesh, interpolate flow values to the exact droplet location, and advect the droplets under the influence of forces such as drag. Additionally, further complex models can be included such as those for secondary breakup processes. There are three primary steps used within this method: a droplet search, an interpolation, and an integration. A droplet search is performed to determine the location of each droplet with respect to the mesh at every time step. This process iteratively determines whether or not a given droplet lies within a guessed cell. Droplets are said to lie within a given cell if it lies in the interior of the cell, or on one face, edge, or vertex of the cell. The method determines which of the neighboring cells may contain the droplet and then proceeds to evaluate those cells as the potential location of the droplet. In order to improve the efficiency with which this iterative step is performed, the initial guess for a given time step is the location of the droplet at the previous time step.

After the cell containing the droplet is located, solution data is interpolated to the exact location of the droplet. Trilinear interpolation is used to accomplish this. This method however, can only be used for cubic cells, so the hexahedral mesh cells must first be re-mapped to a unit cube. The isoparametric form for the hexahedral coordinates are used for this interpolation as seen below:

\[
f = a f_1 + a f_2 \cdot \varepsilon + a f_3 \cdot \zeta + a f_4 \cdot \eta + a f_5 \cdot \varepsilon \cdot \zeta + a f_6 \cdot \varepsilon \cdot \eta + a f_7 \cdot \zeta \cdot \eta + a f_8 \cdot \varepsilon \cdot \zeta \cdot \eta
\]  

(3.37)

where the new map is a unit cube and therefore \(0 \leq \varepsilon, \zeta, \eta \leq 1\). Each value of the coefficient \(a\) is dependent on both the value of \(f\) for a given variable and for which of the eight vertices of the hexahedron is being considered. The determination of these coefficients can be done using the known values of \(f\), leading to a system of eight equations that can be solved by an iterative method to determine \(\varepsilon, \zeta, \) and \(\eta\). The integration step for the droplet velocity can be performed using Taylor series expansion for the governing equation written as follows:

\[
\frac{d \vec{v}^{n+1}_p}{dt} = f_d(\vec{v}_p, \vec{v}^{n+1}_p) + \vec{f}_g
\]  

(3.38)
This equation can be expanded to the following:

\[
\vec{v}_{n+1} = \vec{v}_n + \left[ \vec{f}_d(\vec{v}_n, \vec{v}_{n+1}^p) + \vec{f}_g \left( \frac{1}{\Delta t} - \frac{\partial \vec{f}_d}{\partial \vec{v}_n} \right)^{-1} \right] (3.39)
\]

The displacement of the droplet can be similarly derived by Taylor series expansion as shown below:

\[
\frac{\vec{x}_{n+1} - \vec{x}_n}{\Delta t} = \vec{v}_{n+1}
\]

(3.40)

\[
\vec{v}_{n+1} = \vec{v}_n + \frac{d \vec{v}_n}{dt} \Delta t
\]

(3.41)

\[
\vec{x}_{n+1} = \vec{x}_n + \vec{v}_n \Delta t + \frac{1}{2} \left( \vec{a}_n \Delta t^2 \right)
\]

(3.42)

where

\[
\vec{a}_n = \frac{\vec{v}_{n+1} - \vec{v}_n}{\Delta t}
\]

(3.43)

The above equations are solved for every droplet over each time step in order to determine the droplet’s displacement. In addition to the above droplet tracking method a secondary breakup model is also incorporated. In high speed flow cases such as those examined herein, the breakup of droplets can eventually be seen to occur due to aerodynamic forces. The work discussed herein uses a modified version of the Cascade Atomization Breakup (CAB) model [39] in which the time at which a droplet breaks up is determined by the Taylor Analogy Breakup (TAB) mode [40]. This methodology and its implementation are discussed at length in [18] and can be summarized as follows. The TAB method is used to predict when a droplet will breakup due to it’s exceeding a critical Weber number at the current time step and also due to the history of the droplet. A history of relative velocities specifically is used to determine when breakup will occur. The TAB model predicts this by solving the equation of motion of a normalized damped, forced, harmonic oscillator using aerodynamic drag, restoring, and viscous forces. This equation is numerically integrated in order to calculate a droplet’s normalized lifetime distortion \(y\). When a value of \(y\) exceeds unity a droplet is said to have broken up. The following algorithm is used to compute this lifetime distortion:

\[
y_{n+1} = \frac{We}{12} \frac{\Delta t}{t_d} (A \cos(\omega \Delta t) + B \sin(\omega \Delta t))
\]

(3.44)

\[
\dot{y}_{n+1} = \frac{1}{t_d} (\frac{We}{12} - y_{n+1}) + \omega e^{-t_d / t_d} (B \cos(\omega \Delta t) - A \sin(\omega \Delta t))
\]

\[
A = \left( y^n - \frac{We}{12} \right)
\]

\[
B = \frac{1}{\omega} \left( y^n + \frac{y^n - \frac{We}{12}}{t_d} \right)
\]

\[
\frac{1}{t_d} = \frac{5 \mu_i}{2 \rho_i r^2}, \omega^2 = \frac{8 \sigma}{\rho_i r^3} - \frac{1}{t_d}
\]
The values of $y^{n+1}$ and $\dot{y}^{n+1}$ are set to zero whenever a droplet is newly injected to the system or created via breakup. From this point on integration continues until the value of $y^{n+1}$ is greater than one, at which point breakup occurs. Following this breakup the parent droplet is split into children where the radius of each child is computed as follows:

$$\frac{r_c}{r_p} = \exp(-K_{br}(We(t_{bu}))t_{bu,r})$$

(3.45)

where $K_{br}$ is a rate coefficient, $t_{bu}$ is the breakup time, and $t_{bu,r}$ is the breakup time for an idealized droplet of the same radius with a constant Weber number over its lifetime. Once the radius of the child droplets is determined, the number of children is determined by requiring the total volume of the children be equal to the volume of the parent. In some situations this leads to an overwhelmingly large number of children. When these situations are found to occur, the children are re-represented as a single parcel and the number of children is recorded.

### 3.5 Eulerian Droplet Tagging

In the liquid jet in crossflow scenario, the liquid injected into a gaseous field undergoes significant changes in structure. In order to gather additional data about the processes that are occurring and the properties of the resulting liquid structures, a method must be implemented to find each individual liquid structure across all blocks of the domain. Gathering of this information also gives way to the ability to seed Lagrangian particles from solution data during runtime. The approach being used is modeled after the methodology developed by Herrmann [22]. This method consists of two primary steps: an in-block identification of structures as a field property and a global reduction of structures that cross block boundaries.

First, within the in-block portion, a cell with a liquid mass or volume fraction above a given threshold is located and given a locally unique identifier. Then, neighboring cells are recursively searched and given the same identifier until the threshold condition is no longer met. This process continues until all cells in the block above the given liquid threshold are identified. During this in-block portion, a list of the properties associated with each locally unique identifier is also generated. The steps taken to perform this in-block step are outlined in Figure 3.1. Figure 3.2 shows a centerplane cross-section contour of the locally unique identifier across several blocks. From this figure, it can be seen that structures across block boundaries have not yet been identified as a single structure. This is especially clear within the body of the liquid jet, where segments are seen to have differing identifiers obviously along planar block boundaries. Further, it can also be noted that several individual structures downstream of the jet have the same local identifier despite not being connected. The latter issue is resolved by the creation of a globally unique identifier for each liquid structure. This globally unique identifier is created by shifting the local identifier by a block-number-related offset.

Once a globally unique identifier is generated in every block, a global reduction of liquid structure identifiers is performed. Since our identifier is created as a field property, passing its information
between neighboring blocks as a boundary condition is accomplished using the same MPI routines as used for the other fluid quantities. Then, by comparing boundary and interior cells along each block face, a reduction is made in any space where two unequal identifiers meet with a smaller identifier value in the boundary cell. When this condition is met, all interior values matching the cell being considered are updated to the lower boundary cell value. By performing a reduction with these rules recursively, structures can be joined across any arbitrary number of blocks. The steps taken to perform this global reduction step are outlined by the algorithm shown in Figure 3.3. Figure 3.4 shows the same cross-section contour as above, now reduced to globally unique identifiers using this methodology. In this figure it is now clear that the jet structure has been unified under a single
while an identifier has changed
Update ghost cell identifiers
for all local blocks do
    for all block faces do
        for all ghost cells with a non-zero identifier
            if ghost cell identifier $i_d_g < $ boundary cell identifier $i_d_b$ then
                for all nodes in local block with $i_d = i_d_b$ do
                    $i_d = i_d_g$
                end for
            end if
        end for
    end for
end for
end while

Figure 3.3 Global Reduction Droplet Tagging Algorithm

unique identifier. Less obviously it can also be noted that individual structures downstream of the jet now correctly have unique identifiers.

Figure 3.4 Global Identifier Centerplane Cross-Section

Once a globally unique field of identifying tags is generated and reduced across block boundaries, a master list of unique liquid bodies is generated from the block level lists. In order to accomplish this, a master list than contains duplicate identifiers is first created. In order to combine these duplicate entries, a heapsort is performed by global identifier on this list. By performing this sort, duplicate identifiers are now neighboring entries in the list, allowing for a much more efficient
search for duplicates. The duplicate entries can than be easily combined into single entries.

Several parameters are gathered for each droplet, including total volume, volume averaged velocities and centroids, as well as an eccentricity measure. As centroids cannot be calculated before the final global master list is assembled, a standard eccentricity calculation evaluating each cell within the structure would be overly expensive. In order to calculate a similar eccentricity value, a bounding box is created for each structure by storing block level maximum and minimum location values in each direction. This bounding box method then uses the location furthest from the centroid, \( d_{\text{max}} \) to evaluate the below eccentricity calculation

\[
e = \frac{d_{\text{max}}}{r_{\text{sphere}}} \tag{3.46}
\]

where \( r_{\text{sphere}} \) is the radius of a sphere with equivalent volume.
4.1 Computational Domains

Domains utilized for the work herein were creating using GridPro (Program Development Company) [41]. All of these domains are structured hexahedral multi-block domains. The meshes are divided into two primary categories, aerated liquid injection into supersonic crossflow and pure liquid injection into subsonic crossflow.

4.1.1 Aerated Liquid Injection into Supersonic Crossflow Domains

The supersonic case grids correspond to the aforementioned experimental work performed by Lin et. al. with the Air Force Research Labs. These specific meshes were created for the supersonic liquid jet in crossflow case [5], with the intent of examining the same cases performed in the experimental work. The supersonic case consists of an 170 mm by 50.8 mm by 50.8 mm crossflow region with a 1.0 mm injector located along the floor of the mesh centered approximately one-quarter of the axial distance of the domain. A coarse mesh containing roughly 8 million cells was first generated for preliminary studies. Figure 4.1 shows the blocking structure of this initial grid.

Following these preliminary examinations, adjustments were made to extend the crossflow region inlet by 70 mm in order to allow for the development of a turbulent inflow condition to more accurately match the wind tunnel results. This new mesh was also created with a much finer resolution, increasing the number of cells by an order of magnitude to approximately 108 million cells. Figure 4.2 below shows the blocking structure of this refined grid. Figure 4.3 shows a cross-sectional close up of the blocking arrangement near the injector face with regions inside the injector highlighted in red.
4.1.2 Liquid Injection into Subsonic Crossflow Domains

The second type of domain utilized in this work was a highly Cartesian mesh with a large isotropic section located in the primary breakup region of the liquid jet. These domains are based on work presented originally by Xiao et al. [42]. These meshes do not contain a physical injector and only consist of a 0.03m by 0.0254m by 0.0254 crossflow section. Instead of a meshed injector, these cases used a patch boundary condition representing an injector face with an exit diameter of 1.0 mm. The
isotropic region of the mesh extends from just before the injector at 0.0 m until 0.011 m, from the floor of the domain to 0.013 m, and from -0.002 m to 0.002 m in the transverse direction. Within this region, isotropic cell widths of $4\times10^{-5}$ m and $2\times10^{-5}$ m for the coarse and fine meshes are present. A centerplane view of the blocking structure for this mesh is shown in Figure 4.4 where the location of the injector face is within the red box.

### 4.2 Injector Boundary Conditions

In the supersonic crossflow cases, the aerated-liquid jet was supplied through a patch boundary condition representing the outlet of the injector. The conditions supplied to this patch inflow were generated using a pre-computed transient solution for the flow within the injector. Data was extracted along the injector face from this solution and was then mapped onto the matching block faces within the crossflow domain (shown in red in Figure 4.3). In the isotropic mesh cases a different patch boundary condition was used to emulate an injector in place of a fully meshed injector. Within the location that would serve as the outlet face of the injector (within 0.5 mm of the location $x = 0.0007$ m, $y = 0.0$ m, $z = 0.0$ m), an injection boundary condition is enforced. This boundary condition is applied as a pure liquid jet inflow with a velocity and pressure of 8.6 m/s and 1.02 atmospheres respectively.
4.3 Experimental Setup

4.3.1 Supersonic Experimental Setup

The aforementioned supersonic cases were examined experimentally in works performed at Air Force Research Laboratory, Wright-Patterson Air Force Base. Several experiments were performed to study liquid jet in crossflow behavior for various injectors, injection conditions, and crossflow conditions. A large open loop supersonic wind tunnel was used to generate a crossflow at Mach 1.94, as described in [43]. An axisymmetric injector with an outside-in aerating body was used to create a water-nitrogen aerated liquid jet normal to the tunnel flow. Two nozzles, both with an $L/d_0$ of 10, were examined, one with a converging nozzle and the other converging-diverging (C-D). The constant diameter nozzle had an exit diameter of 1.0 mm. The C-D nozzle featured a 1.0 mm throat with 2.0 mm diameter entrance and exit. The injector was mounted either flush with the floor or raised 7.9 mm into the crossflow. Gas-liquid ratios (GLRs) from 0 to 6% were studied with a constant liquid mass flow rate of 18.2 g/s. Two types of measurements were performed for these cases: shadowgraph imaging and phase Doppler particle analysis (PDPA) with which information regarding the evolution of the liquid jet as well as information about the droplet size, velocity, and volume flux was measured [5]. The present work considers only the converging nozzle at a GLR of 4%.
4.3.2 Subsonic Experimental Setup

The above mentioned subsonic liquid jet in crossflow cases are discussed in qualitative comparison to work done by Sallam et al. in [7]. This effort utilized pulsed shadowgraph and holograph observations in order to determine breakup properties as a function of many parameters. The present studies are concerned with the observable phenomena for a regime dubbed shear breakup in the experimental work. Sallam used the criteria of a Weber number, or the ratio of interial to surface tension forces, to differentiate between breakup regimes of liquid jet into crossflow scenarios. The definition used by Sallam for Weber number is also used within this work and is as seen below:

\[ We = \frac{\rho g d_{jet} u_{\infty}^2}{\sigma} \]  

where \( d_{jet} \) is the diameter of the jet, \( u_{\infty} \) is the free-stream velocity of the crossflow, and \( \sigma \) is the surface tension. These works utilized either a 610 mm x 610 mm subsonic wind tunnel or a shocktube to generate crossflows across a wide range of velocities. Round nozzles with diameters ranging from 0.5 to 2.0 mm were mounted to inject round non-turbulent liquid jets downward into the crossflow in both crossflow apparati. Single-pulse shadowgraphy techniques were used for both systems to image the flow fields. Additionally an off-axis holographic camera setup was used to provide a field of view of 25 mm in diameter at the initial liquid column location. Double-pulsed holograms were then used to derive liquid velocities. These experiments contain a wide range of test cases for multiple liquids over a wide range of Weber numbers that include those relevant to the effort herein.

Additional comparisons are also made briefly to the experimental works of Wu et al. [44] and Elshamy [45]. Both of these efforts examine the breakup of liquid jets in subsonic crossflows under various conditions. One case from each is used as the basis for qualitative comparisons. The specific conditions for each of the conditions are discussed later when the comparisons are made. The effort of Wu et al uses similar methods to those used by Sallam et al. Liquid injection is made through the floor of a subsonic wind tunnel at various conditions using various injectors. A double pulse shadowgraph imaging technique using a laser with 532 nm pulses as a light source is used to capture the near-field breakup of the liquid jet. The effort of Elshamy uses a planar laser scattering imaging technique in place of shadowgraphy. This technique utilizes laser light scattering from the liquid bodies that is then collected by a camera. The data recorded by this method can than be post-processed to create images of the liquid jet as it undergoes breakup.
5.1 Aerated Liquid Injection into a Supersonic Crossflow

In this section the results obtained for the injection of an aerated liquid-gas mixture into a supersonic crossflow originally presented in [18] and [17] are discussed and compared to available experimental results [5]. This case discusses an Eulerian-Lagrangian approach utilizing large-eddy simulations of the spray development from the injection process paired with the previously described Lagrangian particle tracking methodology. An aerated liquid-gas mixture with a gas-liquid ratio (GLR) of 4% and a liquid mass flow rate of 18.2 g/s was injected through a 1 mm diameter straight-nozzle into a Mach 1.94 crossflow at a temperature of 300K with an ambient pressure of 26.4KPa. As discussed above, a time-dependent boundary condition is applied over the faces that connect the aerated-liquid injector to the crossflow portion of the domain. This inflow condition was generated by earlier LES simulations of the injector itself.

Two approaches for the initial distribution of droplets are explored in this study: a core-annular distribution and a log normal distribution. In both cases, the number of droplets introduced at each time step is such that the total volume of liquid injected at the inflow plane is converted to

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crossflow Mach Number</td>
<td>1.94</td>
</tr>
<tr>
<td>Ambient Temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Ambient Pressure</td>
<td>26.4 KPa</td>
</tr>
<tr>
<td>Injection Liquid Mass Flow Rate</td>
<td>18.2 g/s</td>
</tr>
<tr>
<td>Injection Gas-Liquid Ratio</td>
<td>4%</td>
</tr>
<tr>
<td>Nozzle Diameter</td>
<td>1 mm</td>
</tr>
</tbody>
</table>
an equivalent population of droplets. In the core annular case, the droplets are sized in a bimodal fashion such that the core is assumed to consist of 10 micron droplet and the annulus 20 micron droplets. In the log-normal distribution cases, the total volume is distributed in a log-normal fashion with a mean of 7.5 microns and a standard deviation in the logarithmic coordinate of 0.5. An example of both of these initial distributions is shown along the injector face in Figure 5.1. The droplets are then assigned the velocity of the continuous field. In some cases, breakup is modeled using the aforementioned Taylor Analogy Breakup and modified Cascade Atomization Breakup model.

![Initial Lagrangian Droplet Distributions Along Injector Face](image.png)

**Figure 5.1** Initial Lagrangian Droplet Distributions Along Injector Face

### 5.1.1 Preliminary Study

First, a preliminary case was run using a coarse grid with a laminar crossflow inlet condition. Figure 5.2 below shows the instantaneous and time averaged vapor mass fraction, as well as an overlayed instantaneous group of droplets, all along the transverse center plane for this preliminary case. A subset consisting of every 50th particle is shown from the total of approximately 10 million droplets at steady state. Lagrangian droplets seeded for this case consisted of the bi-modal core-annular distribution discussed above. As these droplets follow a mixture relative velocity definition, and the vapor mass-fractions are small near the jet exit, the drag forces are higher resulting in the droplets closely following the mixture field as it expands. As the droplets penetrate further into the crossflow region they no longer follow the mixture plume as closely but rather drift towards its outer edges as drag forces diminish. This drift towards the outside of the plume impacts the 20 micron droplets much more so than the 10 micron droplets as seen in Figure 5.3.

Significant simplifications were made for this early study. It can be seen from the instantaneous piece of Figure 5.2 that small individual structures are not being adequately captured; this is not entirely unexpected, as the overall resolution of this mesh is rather small with only about 10 million
5.1.1.1 Comparison with Experimental Data

Despite the already clear needs for greater mesh resolution, initial comparisons were made with the PDPA data obtained by Lin et al. [5] as an early attempt at validation. These comparisons were made by binning droplet data within 2 mm x 0.5 mm x 0.5 mm volumes along the plane being examined. Averages were than taken for all Lagrangian droplets within each zone, after which the process was repeated and time-averaged over forty-five total time steps. Figures 5.4 and 5.5 below show this comparison for axial and transverse velocities. From these images, it is apparent that the vertical extent of the plume is under-predicted in this preliminary case. In regions where the PDPA data is available, the axial velocity values are in good agreement with the experiment. The vertical velocity component however is not and the computational data under-predicts the experimental results by about a factor of 2. While there is some marginal agreement with the experimental results in this
early portion of the study, a more physically accurate simulation is still obviously necessary.

5.1.2 Refined Study

In order to better examine this problem, a more suitable mesh was created. This mesh increased the number of cells ten-fold as well as incorporated a lengthened crossflow inlet section to accommodate the generation of a turbulent inflow condition. In this case, the previously mentioned log-normal droplet initial distribution was used. This distribution was chosen based on improved agreement for subsonic crossflow cases shown in [17] and [24]. Figure 5.6 shows the instantaneous Mach number at a center-plane in the crossflow direction paired with three slices in the transverse direction. The aerated-liquid jet can be seen to expand outside of the nozzle, both downstream with the flow and upstream just behind the bow shock. A large increase in Mach number would be expected with a free-jet expansion in a perfect gas flow; however, this is not seen here due to the use of the previously mentioned harmonic weighted sound speed and the assumption of isothermal flow. Note that the flow is highly turbulent and that the plume is influenced by eddy structures in the incoming
boundary layer.

Figure 5.6 Supersonic LJICF Instantaneous Mach Number

5.1.2.1 Comparison with Experimental Data

Figure 5.7 shows snapshots of the droplet fields for cases with and without the breakup model discussed in Section 3.4. These results are then compared with experimental shadowgraph data from [5]. In the breakup case, after reaching a statistically steady state, the earlier mentioned parceling technique is used to limit the total number of tracked parcels to about 9 million. In general it is observed that the case with breakup included better agrees with the experimental observations for plume size and shape. This is because the smaller droplets created by the breakup processes more rapidly adjust to the dominant crossflow velocity, achieving less penetration. Less expansion into the crossflow upstream of the nozzle is also seen in the experimental results when compared to either computational case. This upstream expansion is marginally greater in the non-breakup case.

PDPA results were also obtained in the experiments by Lin et al. [5]. By processing time-resolved droplet data as discussed in the preliminary case, the following predictions are shown in Figures 5.9, 5.8 and, 5.10. In these figures center plane axial and crossflow planes at X/D = 100 are shown and compared to PDPA data. These figures compare axial velocity, transverse velocity, and Sauter mean diameter, respectively. In both the experimental data and the computational results, a horse-shoe like axial velocity distribution can be seen. This is a direct result of counter-rotating vorticies created in the injection process. In the computational results, a peak in velocity and Sauter mean diameter occurs nears near the center-plane which is due to the accumulation of larger droplets in this region. Unfortunately, the PDPA data does not extend far enough in the vertical direction to determine whether this is observed in the experiment. In each of these figures, it can be seen that the experimental PDPA data more similarly matches the plume from the computational case in which droplet breakup was not included. When the breakup models are activated the plume is significantly smaller, as the droplets rapidly lose much of their vertical momentum resulting in
noticeably reduced penetration. The aggressive nature of the breakup model can be seen in Figure 5.10, where droplets seeded at the injector face experience very rapid breakup due to the high Weber numbers encountered in the initial expansion of the jet into the crossflow region. After undergoing further secondary breakup events, the resulting plume consists of smaller droplets between roughly 4 and 6 microns in diameter. In the breakup case a similar, although lesser distribution of larger droplets occurs as a peak near the top of the plume at the center-plane. From the PDPA data it is seen however that this distribution of larger droplets occurs along the entire perimeter of the plume and not only the along its top. The rate at which these breakup processes occur is largely dictated by the Weber number distributions experienced in the initial injection process as the jet enters the crossflow. Better models for these initial stages of dense spray injection and perhaps less aggressive breakup models may provide resolution to the differences observed in the computational
and experimental results.

Overall the use of the breakup models described herein does not improve the agreement with the PDPA experimental data. PDPA is more accurate when the spray is less dense, as such, the measurement may preferentially sample the larger droplets that populate the outer fringes of the plume. The shadowgraph imagery shown in Figure 5.7 suggests that the core of the plume is densely populated by light-scattering droplets. These droplets follow the flow more closely and therefore must be smaller than their counterparts in the perimeter region. This trend is better matched by the computational result which includes breakup models but, the almost absolute lack of droplets above 10 microns seen with this result is unrealistic.

5.2 Pure Liquid Injection into a Subsonic Crossflow

The second portion of the effort presented herein involves the study of a pure-liquid jet in a subsonic crossflow. Unlike in cases that involve aerated-liquid jets, pure-liquid jet phase interfaces can be
### Table 5.2 Pure Liquid Jet in Subsonic Crossflow Simulation Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crossflow Velocity</td>
<td>110 m/s</td>
</tr>
<tr>
<td>Ambient Temperature</td>
<td>298 K</td>
</tr>
<tr>
<td>Ambient Pressure</td>
<td>101325 Pa</td>
</tr>
<tr>
<td>Weber Number</td>
<td>206</td>
</tr>
<tr>
<td>Injection Velocity</td>
<td>8.6 m/s</td>
</tr>
<tr>
<td>Nozzle Diameter</td>
<td>1 mm</td>
</tr>
<tr>
<td>Liquid Density</td>
<td>993.5 kg/m$^3$</td>
</tr>
<tr>
<td>Liquid Viscosity</td>
<td>8.93x10$^4$ kg/(m-s)</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>0.072 N/m</td>
</tr>
</tbody>
</table>

well resolved outside of the nozzle. As such this second portion is largely focused on the use of sharp-interface capturing techniques. With this in mind, a mesh was created similar to the one used by Xiao et al. in [42] and described earlier in Section 4.1.2. The critical change in this mesh was the inclusion of a geometrically isotropic region at the center of the mesh. In order to develop this near fully isotropic region, no injector region was included in the mesh. Instead of an injector inflow condition imposed at specific block faces as in the previous study, the injector inflow was imposed in cells along the bottom of the domain within the appropriate radius of a predefined "nozzle" center. From this boundary-defined injector face, a pure liquid jet was injected at a velocity of 8.6 m/s into a crossflow with a free-stream velocity of 110 m/s. Considering the liquid as water and the crossflow as air, a jet diameter of 1 mm leads to a Weber number for this case of approximately 206.

In this case, the primary area of investigation is the ability of the different sharp interface capturing schemes in Section 3.3 to accurately and crisply resolve small liquid structure details. Several interface capturing options are examined, including the baseline PPM reconstruction, two implementations of a THINC scheme, and a BVD scheme. Comparisons between the computational results from this study and experimental results of Sallam et al. [7] are also made qualitatively to confirm that the expected physical phenomena are seen in our simulations. Finally, unique liquid structures are identified and the results used to assess the performance of some of the interface tracking schemes.

### 5.2.1 Comparison with Experimental Data

The effort of Sallam et al. [7] to define and study breakup modes for non-turbulent round liquid jet into crossflow type problems is used as a basis for confirming the capturing of expected physical phenomena. In this study, regions are defined for breakup modes based on Weber numbers. Sallam
defines five primary regions as outlined below:

\[
W e = \begin{cases} 
0 & \text{No Breakup} \\
0 < We \leq 4 & \text{Column Breakup} \\
4 < We \leq 30 & \text{Bag Breakup} \\
30 < We \leq 110 & \text{Multimode Breakup} \\
110 < We & \text{Shear Mode Breakup}
\end{cases}
\]  

(5.1)

By this standard, the case examined herein should represent shear breakup of a liquid jet. Figure 5.11 show shadowgraph images from the work by Sallam et. al. capturing the expected phenomena over the range of breakup modes. From right to left these images show the cases of: \( We = 0 \) no breakup (a), \( We = 3 \) column breakup (b), \( We = 8 \) bag breakup (c), \( We = 30 \) multimode breakup (d), and \( We = 220 \) shear breakup (e). This image is shown for the purpose of discussing Weber number based breakup modes; while this image shows similar Weber numbers to those in this study, the experimental case does not use the same liquid jet or crossflow conditions as the works herein. For the purposes of the studies performed herein it is expected that the breakup phenomena observed would most resemble the fully shear breakup case at \( We = 220 \), but conditions such as jet penetration will not be consistent. Figure 5.12 below shows the first results of this study, a piecewise parabolic method solution with no additional sharp interface capturing reconstruction. This figure shows a side view of an isosurface generated at the phase interface. In comparing this result to that of image (e) in Figure 5.11 we can note some similarities and differences in the structures. The most obvious difference between these two results is the lack of the small droplet cloud appearing on the downwind side of the jet in the computational case. When searching for the same feature in a lower Weber number experimental case (image (d) of Figure 5.11), the droplet cloud in this area is considerably less dense but still denser than is captured in this single frame solution. Another area
for comparison to the shear breakup mode is the presence of wave-like instabilities that originate near the base of the jet and grow in magnitude as the jet penetrates the flow. These are clearly seen in image (e) above but are noticeably less defined in image (d). Figure 5.13 examines more closely the base of the jet in the computational result. Small disturbances can be seen developing within one nozzle diameter of the injection face. These disturbances grow along the upwind side of the jet until the point where large liquid structures begin to break from the jet. As these large structures break off into ligaments, they terminate at their end with the formation of a droplet, which is expected in this breakup regime. However, it would also be expected that these droplets and ligaments grow in diameter with the growth of the surface instabilities. This trend does not concretely appear in this result because while the ligaments do tend to grow with the flow of the jet, finer droplets breaking from ligaments are not seen nearer to the injection point.

Figure 5.14 shows a comparison between a similar PPM solution isosurface and two experimental works by Wu et al [44] and Elshamy [45]. Neither of these experimental cases matches the conditions of the computational experiment exactly; however, both are in similar breakup mode regimes. Table 5.3 shows the conditions for each case. Both experimental cases occur a lower Weber number resulting in greater penetration of the liquid jet compared to the computational result. Similar overall behaviors can be seen between the three images, a primary liquid column breaking into medium sized liquid structures and further into ligaments and droplets. However, the computational results are missing the high-density clouds of small droplets downwind on the primary jet body. As the computational results show a higher Weber number flow, this lack of catastrophic breakup is even more critical.

Other efforts have been made to examine similar problems using computational fluid dynamics.
**Figure 5.13** Pure Liquid Jet into Subsonic Crossflow PPM Isosurface Closeup

**Table 5.3** Pure Liquid Jet in Subsonic Crossflow Simulation Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Computational</th>
<th>Wu et al. [44]</th>
<th>Elshamy [45]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weber Number</td>
<td>206</td>
<td>139</td>
<td>100</td>
</tr>
<tr>
<td>Injection Velocity (m/s)</td>
<td>8.6</td>
<td>9.3</td>
<td>8.8</td>
</tr>
<tr>
<td>Crossflow Velocity (m/s)</td>
<td>110</td>
<td>68.6</td>
<td>63.9</td>
</tr>
<tr>
<td>Nozzle Diameter (mm)</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

**Figure 5.14** Pure Liquid Jet in Subsonic Crossflow Comparison to Experiments of (a) Wu et al (Shadowgraph) [44] and (b) Elshamy (Planar Light Scattering) [45]

Xiao et al [42] examines various Weber numbers, injector diameters, and other problems for pure liquid jets in subsonic crossflows. Figure 5.15 below shows a comparison between the results of Xiao's efforts on the left, in orange and the PPM results from this effort on the right, in blue. Clearly, the results of the PPM method lack the large numbers of small droplets and liquid structures captured by Xiao et al. Plume shapes are relatively consistent between the two cases, with the results of the effort herein showering slightly less penetration by the primary jet body. Both results again show the
presence of surface wave instability at the base of the liquid jet. These instabilities have substantially
greater magnitudes in the work of Xiao et al, which is likely a driver for the more violent breakup
seen in comparison to the results of the efforts herein.

Figure 5.15 Pure-Liquid Jet into Subsonic Crossflow Comparison with Efforts by Xiao et al (Left) [42]

From the presence of the defining features of both surface instabilities and the formation of
large ligaments that breakup into smaller droplets, it can be determined that this case is correctly
falling in the shear breakup regime. When compared to various experimental and computational
studies this case; however, has not fully captured smaller liquid structures formed from the surface
instabilities and termination of ligaments. From this brief qualitative comparison we are able to
ascertain that while this case is correctly in the shear breakup regime, the ability to better capture
smaller fine details of phase interfaces is needed.

5.2.2 Comparison of Phase Interface Reconstructions

The above case illustrates the issue of the inability to capture well the fine details of the liquid jet in
crossflow problem. In this section, attempts are made to improve on this problem by incorporating
sharp interface capturing schemes listed above in Section 3.3. These schemes are primarily of the
tangent-hyperbola interface capturing (THINC) type, which seek to model sharp interfaces within a
mesh cell by using a hyperbolic tangent function. Three such schemes will be compared throughout
this section; Case A the time dependent THINC scheme, Case B the time independent THINC
scheme, and Case C which utilizes the same scheme as Case B but at a one-half reduced time-step.
In addition to these three schemes, the above PPM results will also be shown in comparison when
applicable.

Figure 5.16 shows isosurfaces generated from the 50% contour of the volume fraction, all of
which were generated for only the isotropic region of the mesh. The first observation of note is the
increased magnitudes of the instabilities forming along the upwind side of the jet in all of the sharp interface capturing schemes when compared to the PPM solution. As is expected these increased magnitudes lead to faster and more violent breakup of the primary liquid jet structure. In the PPM solution the surface waves forming along the upwind side of the jet do not grow significantly until large liquid bodies begin to break away. In the sharp interface capturing solutions surface waves grow much faster along the main body of the liquid jet. Another area of interest is the formation of thin ligaments terminated by small droplets close to the injection point, a trait which was noticeably absent in the PPM solution. These thin ligaments can be seen in the solutions of all of the sharp interface capturing schemes. The formation of small droplets from these ligaments, however, is less apparent in Case A. An increased number of small structures can also been seen in the sharpened solutions, though most of these small structures are contained within a smaller overall plume shape than shown for the PPM scheme. The differences in Cases B and C are minimal, which is expected as the same scheme is utilized with only varying time-step sizes. An injector face closeup view of these isosurfaces can be seen in Figure 5.17. From these images, it is clear that surface instabilities begin nearer to the base of the jet in the THINC reconstructions, beginning nearest to the injection face in Case B. The evolution of these initial surface waves into more influential disturbances and shape changes can also be seen.

Figure 5.18 shows instantaneous centerplane contours of vapor volume fraction at three time levels for each of the schemes considered. Very similar behavior of the liquid jet breakup process can be observed in these images. First, a large structure breaks from the primary jet, followed by the breakup of that structure as it moves with the crossflow. Surface waves can also be seen growing along the upwind side of the liquid jet in each of the cases, with the greatest magnitudes seen in Cases B and C. Case A also shows this phenomena, but at a much smaller magnitude than is seen in the other cases. In the downstream region, numerous small liquid bodies can be seen in Cases B and C. These small structures are lesser in number in Case A.

Figure 5.19 shows isosurfaces over 70 frames (1.75 \times 10^{-4} \text{ seconds}, 0.65 flow through times) overlaid on themselves. Taken together, these images indicate the time averaged extent of the plumes. In these images, a narrower plume is seen for all of the sharp interface capturing schemes when compared to the PPM solution. Minor differences in the resulting plume shape can be noticed between the sharp interface capturing schemes. The plume, for example, is most narrow in Case A, which also shows the greatest penetration of the liquid jet. Case B shows the shallowest penetration height of the THINC schemes, with Case C falling between A and B. These differences in penetration are relatively small (less than 1.5 mm) between Cases A and B. Cases B and C differ more than has been noted until this point, with Case B showing a wider and less dense plume core when compared to Case C. Additional comparisons of the plume shape can be seen in time-averaged mass fraction contours in Figure 5.19. From these contours, penetration heights are seen again to be very similar. Plumes are narrower in height in Cases A and B. The plumes are also denser at their core in plumes B and C than in Case A. The core of the plume in Cases B and C also begins slightly lower than in Case A which may be representative of breakup beginning closer to the injection point. As expected
Figure 5.16 Isosurface Comparison of Interface Sharpening Schemes
Figure 5.17 Sharp Interface Capturing Scheme Comparison Closeup View
Figure 5.18 Sharp Interface Capturing Scheme Vapor Mass Fraction Contour Comparison
the differences between Cases B and C are again minimal, as they utilize the same scheme only varying the time-step size.

Figure 5.19 Sharp Interface Capturing Scheme Isosurface Plume Shape Estimate

Figure 5.20 Sharp Interface Capturing Scheme Time Averaged Mass Fraction Plume Shape Comparison

5.2.3 Mesh Refinement

A second refined mesh was created to evaluate the effects of grid resolution on the overall ability to capture the sharpness of interfaces and details of the breakup process. Figure 5.21 shows a side view of the isosurfaces created for the Case B scheme for both the coarser and finer mesh at a
50% vapor volume fraction. In these images, the more rapid breakup and development of smaller droplets can be observed, resulting in a much larger and denser cloud of small droplets. The large liquid structures breaking from the main jet are also smaller in size when compared to the coarse mesh case. Also of note are the much thinner ligaments forming on the downwind side of the primary jet in the refined mesh case. Figure 5.22 shows closeup views of these two isosurfaces which better show the formation of these thin liquid tendrils. It can also be more clearly seen in the finer mesh that these thin liquid structures terminate with the formation of droplets. Figure 5.23 shows

Figure 5.21 Mesh Comparison Isosurface for 50-percent Vapor Volume Fraction

Figure 5.22 Mesh Comparison Isosurface for 50-percent Vapor Volume Fraction Detail
instantaneous snapshots of vapor phase mass fraction along the centerplane of the domain for each mesh density. As would be expected, the fine mesh solution shows far smaller liquid bodies with less smeared interfaces present. An increased number of overall liquid bodies is also present in the finer mesh case. This result serves to affirm the notion that smaller cells may better capture the catastrophic breakup processes involved in shear breakup as this denser cloud of smaller droplets better agrees with the experimental observations discussed above. The magnitude and frequency of the surface waves along the upwind side of the jet is fairly comparable between the two mesh densities. Figure 5.24 shows a comparison of the time-averaged vapor mass fraction between the two mesh densities. These time-averaged contours show that the fine mesh study produces a plume than penetrates roughly 1mm less. The core regions of the two plumes however, are more similar in maximum penetration height. The core region of the plume in the finer case also begins at a slightly lower height from the floor of the domain. A narrower primary jet body is also seen in the fine resolution case. Overall the refined mesh case shows significantly sharper phase interfaces which may explain many of the observed differences. A sharper interface along the top of the plume leads to less smearing and the plume edges appearing close to the core, reducing maximum penetration. Similarly, the increased ability to capture small droplets noted above is a potential cause for the growth of the core downward as the mesh is refined.
5.2.3.1 Comparison of Reconstructions

The below Figure 5.25 shows isosurfaces at a volume fraction of one-half for both the THINC Case B and BVD schemes. It is highly apparent that the results from the BVD scheme are more diffusive, forming much smoother liquid structures. The primary liquid jet body does not break up as quickly in the BVD case, resulting in pockets of liquid that are only partially broken free from the main column. It is also apparent that many small and mid-sized liquid structures present in the Case B results are absent from the BVD result. Figure 5.26 shows a close up of the two isosurfaces nearer to the injector face. The initial instabilities along the jet column appear in greater frequency in the THINC solution. The ligaments that form as a result of these instabilities are also absent in the BVD case. Overall the isosurfaces generated for the two reconstructions show that the THINC scheme captures smaller ligaments, droplets, and surface details than in the BVD case.

Figure 5.27 shows time averaged vapor mass fraction contours for both schemes along the transverse centerplane. The BVD case shows both an increase in penetration and a denser core when compared to the THINC scheme results. This is expected based on the above isosurfaces where breakup of the primary jet is limited in the BVD case. The larger structures captured in the BVD case are slower to turn with the crossflow resulting in the increase in penetration. Figure 5.28 shows the evolution of the vapor volume in three time-steps - comparable to Figure 5.23(b). In comparing these two figures, it is obvious that far fewer small structures are captured when utilizing the BVD reconstruction. The structures that are captured with the BVD scheme are less crisp, especially as they continue downstream. All of these comparisons show a consistently more diffuse result in the BVD solution than in the THINC solution.
5.2.4 Droplet Tagging

The final area of analysis for this liquid jet into subsonic crossflow study is the evaluation of quantitative data obtained from a newly implemented droplet tagging methodology. This method, discussed at length in Section 3.5, allows for the identification and categorization of unique liquid structures throughout the entire domain. While many parameters may be extracted using this method, the two that are focused on herein are the volume of each structure and its eccentricity. These two parameters are chosen as an area of focus for this study as the eventual goal of this new piece of software is to identify small droplets and transfer them as seeding parameters to the Lagrangian particle framework discussed earlier in this document. In order to choose the correct droplets to transfer, they must be sufficiently small and round to be modeled accurately as spheres.
5.2.4.1 THINC (Case B)

The result of the Case B scheme on the refined mesh are first analyzed using this method. Twenty-five frames of data taken 250 iterations or 0.125 milliseconds apart are extracted for unique structures and their properties. The average number of droplets found in this case in each frame was approximately 1500. The sum of these liquid structure entries are then binned and used to create the following histograms for volume and eccentricity. One-dimensional histograms of volume and eccentricity are seen in Figures 5.29 and 5.30 respectively. Volumes are binned in a logarithmic scale and eccentricities in a linear scale. In Figure 5.29, an almost log normal distribution of volumes can be seen centered roughly about the volume $2 \times 10^{-15}$ m$^3$. The notable exceptions to this normal distribution come at the smallest volume bins where large spikes between volumes of $4 \times 10^{-15}$ m$^3$ and $1 \times 10^{-14}$ m$^3$ can be seen. The large increases in probabilities for this range is likely the result of the mesh resolution as these scales are at or near to the smallest cell volumes. The probability distribution for eccentricity seen in 5.30 is similar to that of the volumes. The distribution is again normal with the exception of outliers at eccentricities below one. These values below one are physically undefined and are a result of the rough estimation technique used for eccentricity at
this time. The largest outlier comes at an eccentricity of zero can be explained by the fact that the eccentricity is calculated using only cell centered coordinate locations, meaning that when a droplet falls within a single cell, its center and boundary are defined as the same point. The second set of outliers nearest to an eccentricity of one can be similarly explained. The possibility for a spherical droplet of equivalent volume that is larger than the distance from the centroid to the furthest cell center exists as cells may contain a liquid volume fraction of greater than one-half. As the mesh cells are small, it is expected that the ratio of the actual and ideal droplet radii are similar, resulting in eccentricities near to but below one. This result is confirmed by the existence of peaks in the histogram just below an eccentricity of one that do not continue to appear at lower values. The normal piece of this distribution is centered above an eccentricity of 1, at approximately 1.75. This is the expected result in a flow that contains both the formation of spherical droplets and ligaments as well as a large primary jet structure.

Figure 5.29 Liquid Structure Volume Histogram for Case B

A third three-dimensional histogram shown in Figure 5.31 is used to show the dependencies between eccentricity and volume. From this figure it can be noted that the bulk of liquid structures fall mostly in the range of eccentricities between 1 and 2.5 and volumes between $3 \times 10^{-14}$ m$^3$ and $1 \times 10^{-12}$ m$^3$. Also notable in this figure is the general trend of higher eccentricities for higher volumes and vice versa. Another observation made from this figure is the gap located between the peak values for volume and the bulk of the fluid structures. These bins in the histogram represent the primary liquid jet which is both highly eccentric and significantly larger than other structures in the domain. Finally it can be seen that the zero eccentricity values do correspond to the smallest
Figure 5.30 Liquid Structure Eccentricity Histogram for Case B

volumes captured by this method, affirming the suspected reasonings mentioned above.

Figure 5.31 Liquid Structure Eccentricity Histogram for Case B

Figure 5.32 shows an orthographic projection of the distribution of the droplets captured with this method scaled and colored by the logarithm of the volume as a three-dimensional distribution over the computational domain at one time frame. From this it can be seen that a core of larger volume bodies exists that is surrounded by and interspersed with smaller droplets. This is expected of a shear breakup mode as many rapid breakup events should occur in quick succession stemming from the jet. The rear view in this figure (shown in the bottom left) also shows the structure categorized as the main jet as the singular body at the red end of the colorscale.

Similarly, Figure 5.33 shows the same projection but colored and sized by eccentricity. The most
A meaningful observation from these images is the existence of a highly eccentric core shedding into more spherical droplets. This result is expected when considering the physical behavior of a jet in shear breakup, in which the jet sheds into highly eccentric ligaments that then break up into rounder droplets.

By overlaying several of the above droplet data sets for different time frames on each other, the evolution of droplets tagged by this methodology can be seen. Figure 5.34 shows every third snapshot.
of the gathered twenty-five frames, scaled and colored by volume. Two important observations are garnered from this figure. First, the droplets tagged by this method are consistently found as they move through the domain. Second, these bodies that have been consistently tagged show evidence of breakup as they tend to become smaller over time.

![Figure 5.34 Multiple Frame Droplet Tagging Data Shown as Particles in a 3D Space - Scaled by Size](image)

Finally, in all the above images concerning the distribution of the liquid structures in three-dimensional space, the same issue is present. That issue is the sudden loss in the number of bodies following the passing of some plane in the crossflow direction. Figure 5.35 shows the mesh blocking structure overlaid on the multi-frame droplet distribution. In this image it can be clearly seen that the loss in tagged structures corresponds with the increase in the aspect ratio of the blocks in the crossflow direction. These skewed blocks contain the gradual lengthening of cells in the same direction. This was noted as a probable issue in the supersonic crossflow case above that is now affirmed with this new technique.

### 5.2.4.2 BVD (Case D)

The above analysis is repeated for the BVD scheme discussed above. Twenty-two datasets were compiled for this case, each taken 250 iterations or 0.125 milliseconds apart. In this case an average of roughly 250 unique liquid structures were found using the droplet tagging, approximately one-sixth of the number captured utilizing the THINC scheme. Figure 5.36 shows a histogram of the logarithm of the volume of the unique liquid structures. Notably absent when compared to the THINC case above is the normal distribution of volumes. Mid-sized structures are not present in significant numbers in the BVD reconstruction solution, leading to a distribution that is heavily dominated by the smallest capturable structures. This lack of mid-sized liquid bodies is likely due
Figure 5.35 Multiple Frame Droplet Tagging Data Shown as Particles in a 3D Space - Scaled by Size

to the smearing of interfaces between structures as they break from the main column. This smearing results in mid-sized bodies that are connected, in some cases by a thin ligament, to the main jet body. The tagging method then considers these to be a piece of the main jet body instead of entirely independent mid-sized structures. When considering the distribution of eccentricities of

Figure 5.36 Liquid Structure Volume Histogram for Case D
the unique structures, Figure 5.37, a normal distribution is captured with the earlier noted outliers again present. When comparing the eccentricity distributions between the two reconstructions, it can be seen that the center of the normally distributed values is slightly larger. Again this is likely due to mid-sized structures failing to fully break away from the main jet body. The zero-eccentricity spike is more prominent in the BVD reconstruction; this is due to the increased number of the smallest capturable structures and the issues with the eccentricity calculation mentioned earlier. A third three-dimensional histogram shown in Figure 5.31 illustrates the dependencies between eccentricity and volume. A similar probability distribution is seen with the BVD results as it was with the THINC results. A mostly linear relationship between volume and eccentricity is observed. This is expected as the larger structures experience greater distortion. It is also obvious from all of these histograms that far fewer unique liquid structures have been captured, especially in the most probable region seen in the THINC case.

Single frame three-dimensional scatter plots of the liquid structures captured by the tagging method for the BVD scheme are shown below in Figures 5.39 and 5.40, scaled and sized by volume and eccentricity respectively. It is immediately obvious that the plume of liquid structures is far less dense than in the THINC results. Although the plumes shown are significantly less dense, the overall behaviors are otherwise consistent. A core of large highly eccentric droplets is surrounded by and interspersed with smaller, less eccentric bodies as was also seen in the THINC reconstruction results.
Figure 5.38 Liquid Structure Eccentricity Histogram for Case D

Figure 5.39 Droplet Tagging Data Shown as Particles in a 3D Space for Case D

Figure 5.40 Droplet Tagging Data Shown as Particles in a 3D Space - Scaled by Size
Numerical simulations were performed for two different liquid jet in crossflow problems: an aerated-liquid jet in a supersonic crossflow, and a pure-liquid jet in a subsonic crossflow. The simulations were performed utilizing the REACTMB-MP solver for the isothermal Navier-Stokes equations. Three primary areas were studied: Eulerian-Lagrangian particle tracking, sharp interface capturing schemes, and an Eulerian droplet tagging method for the extraction of data related to each unique structure. The first study focused on the use of a one-way coupled Lagrangian droplet tracking code to examine droplet distribution and breakup upon the injection of an aerated-liquid jet into a supersonic crossflow. The pure-liquid in a subsonic crossflow study was used to evaluate the differences in several sharp interface capturing schemes and their implementations as well as to develop a method for extracting the properties of unique liquid structures from an Eulerian solution set.

The first case presented herein was the examination of an aerated-liquid jet into a supersonic gaseous crossflow. A preliminary study into this case showed the critical importance of a turbulent inflow condition for the crossflow region, which promoted the breakup of the liquid jet. In this case, Lagrangian particle were seeded using a bi-modal core-annular distribution which was found to predict the plume shape inadequately. Marginal agreement with experimental results was seen for this preliminary case, instigating the creation of a better suited computational domain. In the case of the refined mesh, better agreement was seen with experimental phase Doppler particle analysis (PDPA) and shadowgraph data. In this case, two models were used within the Lagrangian particle tracking framework. The first utilized a log-normal initial droplet distribution and the second used the same initial distribution but also incorporating a droplet breakup model. The breakup model used for these cases was a modified Cascade Atomization Breakup (CAB) model where breakup times were determined using the Taylor Analogy Breakup (TAB) method. The time-averaged plume prediction for the breakup-included case was shown to better match the shadowgraphy images from the experimental studies. However, the opposite was true in comparing with the PDPA data. While both Lagrangian cases were in decent agreement with the velocity profile 100 injector diameters
downstream, the droplet diameter predictions were not. The solution obtained including breakup lacked any droplets with a diameter of above roughly 10 microns. This demonstrated that the droplet breakup models are likely overly aggressive. In all cases, the PDPA data shows a more well defined region of larger droplets in an annulus around a core of finer droplets. This was not seen in the computational results, where a more kidney shaped cap of large droplets was present near the top of the plume. This difference may be partially explained by preferential sampling of large droplets in the PDPA system. Overall the results for the supersonic case were mostly in agreement with the experimental observations; however further work could be performed to analyze discrepancies and paths to resolve them.

The second case presented in this work involves simulations of a pure-liquid jet into a subsonic gaseous crossflow. This portion of the study was primarily focused in two areas: the examination of several sharp interface capturing schemes and the analysis of the initial results from extracting unique liquid structure properties directly from the Eulerian dataset. Two different implementations of tangent hyperbola interface capturing (THINC) schemes were investigated: the first incorporating a local CFL dependence and the second being local CFL independent. In addition, the effect of reducing the time-step for one of the local CFL independent methods was examined. Finally, a boundary-variation diminishing (BVD) reconstruction was incorporated and preliminary results discussed. Overall, the use of sharp-interface capturing schemes was shown to improve the ability of the solver to resolve small liquid structures that should be observed in cases of shear breakup. The surface waves that form on the upwind side of the jet were seen to increase in magnitude when THINC schemes were utilized. A larger increase in this magnitude was shown in the local CFL independent THINC implementations. Additionally, the formation of small droplets and thin liquid tendrils near the base of the liquid jet could be seen in cases utilizing sharp interface capturing methods. As expected the overall number of the smallest droplets captured was increased in these cases as well. In all cases with interface sharpening, the overall plume shape became narrower than in the baseline PPM reconstruction. Dramatic differences were not noticed in the various implementations of the THINC schemes. The BVD scheme provided a significantly more diffusive result, leading to larger smoother liquid bodies and the loss of fine detail when compared to the THINC reconstruction solutions. The BVD solution also resulted in far fewer unique liquid bodies captured when using the droplet tagging system. The results when using the THINC sharp interface capturing schemes were overall seen to better agree with the physical phenomena expected to be present.

Further examination of the subsonic liquid jet in crossflow case was performed utilizing a newly incorporating droplet tagging methodology. This methodology searches the entire computational domain in order to find each unique liquid body and then utilizes field-property data to calculate various properties of the bodies. This method showed that the distribution of the size and eccentricity of the liquid structures mostly followed a normal probability distribution with notable exceptions for the smallest observable droplets as previously discussed. Both of these issues could potentially be addressed by changes to the method used for calculating eccentricity. Of important note is the rapid
loss of liquid structures captured by this method outside of the isotropic portion of this domain. Overall, the use of this new droplet tagging system has proven useful for the evaluation of pure-liquid jet breakup processes.

Mesh resolution dependence studies were also performed for both cases. From this it is readily apparent that a limiting factor in capturing smaller liquid structures is mesh resolution. In the refined mesh cases, both smaller droplets and liquid ligaments were observed in the instantaneous data. Further computational mesh refinements should be performed, given that adequate resources are available, in order to determine the full dependence of the solution on cell size.

Opportunities for future work exist in many areas of this project. Firstly, the results of the supersonic case study were gathered before the study of the various sharp interface capturing schemes and droplet tagging system development, and the subsonic case was never considered using the Lagrangian particle tracking system. The results from the incorporation of these methods in either case may prove useful in better understanding liquid jet in crossflow problems in both a physical and numerical sense. Further, in the supersonic case, it was noted that the droplet breakup schemes considered were likely overly aggressive after comparisons with experimental data. Efforts to examine less aggressive options for driving Lagrangian droplet breakup could be considered. In the subsonic studies, an array of THINC implementations were examined at length for the the coarse mesh case and only one such scheme was deployed on the refined mesh. While the results of these various schemes were largely the same for the coarse mesh case, an opportunity exists to confirm that this holds true independent of mesh resolution. More accurate eccentricity calculation methods should be explored for use in the droplet tagging framework. One option may be to incorporate the reconstruction of the interface within a cell in these calculations; however, that would drastically impact the efficiency of the method. A final key area for improvement on these studies is the removal of the isothermal assumption, which is now possible after the recent addition of the energy equation into the REACTMB-MP solver.

Throughout this project efforts were made to evaluate and further develop the REACTMB-MP flow solver for use in liquid jet in crossflow type problems. These types of problems are of critical importance in the development of scramjet and ramjet fuel injection systems. Cases were examined for liquid jets into subsonic and supersonic crossflows both considering the incorporations of different techniques to better predict and understand the flow field. The results presented herein largely showed good agreement with expected physical phenomena and available experimental data.
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As a wide range of compressibility can exist within multiphase flows, a preconditioning method is used to relax the stiffness of our equation system as the incompressible limit is approached. The method given by Weiss and Smith [46] is followed to produce this matrix. First we consider the standard single phase Euler equations, which have the following eigenvalues:

\[
\lambda_1 = u, \lambda_{2,3} = u \pm a
\] (A.1)

For a normal matrix the condition number can than be approximated as follows:

\[
\kappa = \frac{|\lambda_{\text{max}}|}{|\lambda_{\text{min}}|}
\] (A.2)

Which in the case of the standard Euler equations is then:

\[
\kappa \approx \frac{|u| + a}{|u|} \approx 1 + \frac{1}{M}
\] (A.3)

From the above it can be seen that as the Mach number approaches zero the condition number of the system grows towards infinity leading to very small allowable time steps. These low Mach number flows therefore lead to ever increasing numerical stiffness. In order to resolve this time step limitation some method for to restrict the condition number must be applied. For the work outlined throughout this study the method used by Weiss and Smith [46], based on the Artificial Compressibility (AC) method of Chorin [34] for incompressible flows is used. The derivation of which can is outlined below.

First, for simplicity, the one dimensional Euler equation for two-phase flow is examined, but with an added preconditioning matrix \(P\):

\[
P \frac{\partial \hat{V}}{\partial t} + \frac{\partial \hat{p}}{\partial \hat{x}}
\] (A.4)
Where the preconditioning matrix is expressed as a perturbation of a rank one Jacobian matrix as follows:

\[ P = \frac{\partial \hat{U}}{\partial \hat{V}} + \Theta \hat{u} \hat{v}^T \]  
(A.5)

Where \( \hat{U}, \hat{F}, \) and \( \hat{V} \) are the vectors defined below containing the conservative variables, flux, and primitive variables respectively.

\[ \hat{U} = \begin{bmatrix} \rho_v a \\ \rho \\ \rho u \end{bmatrix} ; \quad \hat{F} = \begin{bmatrix} u \rho_v a \\ \rho u \\ \rho u^2 + p \end{bmatrix} ; \quad \hat{V} = \begin{bmatrix} a \\ p \\ u \end{bmatrix} \]  
(A.6)

To find the eigenvalues of the system we take the following determinant:

\[ \det \left| P^{-1} \frac{\partial \hat{F}}{\partial x} - \lambda I \right| = 0 \]  
(A.7)

The precondition matrix can be defined as:

\[
\begin{bmatrix}
\rho_v & a \frac{\partial \rho_v}{\partial p} + \Theta \frac{\rho_v a}{\rho} & 0 \\
\rho_v - \rho_l & \frac{\partial \rho}{\partial p} + \Theta & 0 \\
u (\rho_v - \rho_l) & u \frac{\partial \rho}{\partial p} + \Theta u & \rho \\
\end{bmatrix}
\]  
(A.8)

In order to solve for the inverse of \( P \) we take its determinant resulting in

\[ \det[P] = \rho \left[ a \rho_l \frac{\partial \rho_v}{\partial p} + \rho_v (1 - a) \frac{\partial \rho_l}{\partial p} + \Theta \frac{\rho_v \rho_l}{\rho} \right] = \rho (\beta + \Theta \gamma) \]  
(A.9)

From which we derive \( P^{-1} \) as follows:

\[
\begin{bmatrix}
\frac{\partial \rho}{\partial p} + \Theta & -a \frac{\partial \rho_v}{\partial p} + \Theta \frac{\rho_v}{\rho} \\
\beta + \Theta \gamma & \beta + \Theta \gamma & 0 \\
\frac{\rho_v}{\rho} & \frac{\rho_v}{\rho} & 1 \\
\end{bmatrix}
\]  
(A.10)
Then multiplying \( P^{-1} \) by \( \frac{\partial \vec{F}}{\partial \vec{V}} \) yields:

\[
P^{-1} \frac{\partial \vec{F}}{\partial \vec{V}} - \Lambda = \begin{bmatrix}
    u - \lambda & \frac{\Theta u \alpha}{\beta + \Theta \gamma} \left( \frac{\partial \rho_v}{\partial \rho} - \frac{\beta}{\rho} \right) & \frac{a \rho_v \partial \rho}{\beta + \Theta \gamma} \\
    0 & \frac{\beta + \Theta \gamma}{\rho} & -\lambda \\
    0 & \frac{1}{\rho} & u - \lambda
\end{bmatrix}
\]

(A.11)

Where

\[
a^2 = \frac{\rho_v \rho_l \rho}{\rho \beta}; \quad \Theta = \left( \frac{1}{V_{\text{ref}}^2} - \frac{1}{a^2} \right); \quad M_{\text{ref}} = \frac{V_{\text{ref}}^2}{a^2}
\]

(A.12)

The eigenvalues of which can than be defined as follows:

\[
\lambda_1 = u, \quad \lambda_{2,3} = \det \begin{bmatrix}
    u M_{\text{ref}}^2 - \lambda & \frac{\rho_t \rho_v}{\beta} M_{\text{ref}}^2 \\
    \frac{1}{\rho} & u - \lambda
\end{bmatrix} = 0
\]

(A.13)

Solving for \( \lambda_{2,3} \) results in the following quadratic expression:

\[
\lambda_{2,3} = \frac{1}{2} \left[ (1 + M_{\text{ref}}^2) u \pm \sqrt{(1 + M_{\text{ref}}^2)^2 u^2 - 4 \left( u^2 M_{\text{ref}}^2 - a^2 M_{\text{ref}}^2 \right)} \right]
\]

(A.14)

Which can than be simplified resulting in the final form of the eigenvalues for this system of equations.

\[
\lambda_1 = u \lambda_{2,3} = \frac{1}{2} \left[ (1 + M_{\text{ref}}^2) u + \sqrt{(1 - M_{\text{ref}}^2)^2 u^2 + 4 V_{\text{ref}}^2} \right]
\]

(A.15)

The condition number of which can be demonstrated to be \( \kappa \approx \frac{1 + \sqrt{5}}{2} \) showing a relaxation of the stiffness of the system and therefore leading to greatly increased allowable time step sizes.
Two primary implementations for tangent hyperbola interface capturing schemes are examined throughout this work. The difference between these two types of THINC schemes is their reliance on a local Courant Friedrichs Lewy (CFL) number which can be seen in 3.3.1. As the time independent THINC schemes are derived directly from taking the limit of the time-step dependent version as the time-step approaches zero, it is necessary to determine the range of time-steps where this assumption is held true. In order to evaluate this dependence a simple one dimensional reconstruction was examined for two schemes (Cases A and B) over a range of time-step sizes. A five cell stencil was used to evaluate the resulting values for each of the two schemes at the left and right faces of each interior cell. While several cases of initial phase fraction values were examined, for brevity the results below all correspond to a single peak in the center cell of 1 where all other cells have been set to 0. The below Figure B.1 shows the average difference in the reconstruction face values for a range of CFL numbers. It is clear from the above that as the CFL number approaches unity, the difference between the reconstructions of the two schemes grows. This difference increases dramatically at CFL values greater than 0.1. However, these differences are incredibly small even at their greatest extents they are still of the order of 1E-9. From this simple analysis the conclusion was made that the time-step independent methods hold valid for the range of time-steps considered within this work.
Figure B.1 1D Comparison of Reconstructions