SIMULATION AND EXPERIMENT OF THE RAPID DECOMPRESSION OF JET PROPELLANT 10

BY

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THESIS

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Abstract

Multiple topics will be discussed in this thesis involving a jet fuel and its equation of state. First, the types of jet fuels, equation of state, and past experiments and simulations will be discussed. Next, the equation of state of Jet Propellant 10 (JP-10) is explained. Furthermore, the effects of exposing JP-10 to high pressures and allowing expansion to occur via nozzle are simulated using a multi-physics simulation program called ALE3D. Specifically, the velocity and shape of high explosive initiated jets of JP-10 will be observed. Also, a parameter study will be performed to see how geometry and other variables effect these results. The simulation results are then compared to experimental results obtained and performed at the University of Illinois at Urbana-Champaign. The experiment is performed with multiple amounts of high explosive, jet fuel, and water for comparison purposes. Lastly, a numerical model will be developed and compared to the simulation results.
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Chapter 1

Introduction

1.1 Overview

Computational simulations offer an inexpensive and more controlled environment compared to experiments. However, computational simulations are only as accurate as the models and material parameters that are implemented into the software. For example, one can only have physically accurate results if the equation of state parameters are properly calibrated. In order to confirm that the initial simulation parameters are accurate, the numerical results need to be compared to experiment results under the same conditions. Once a material’s equation of state parameters are proven to be physically accurate within the simulation, one can proceed with in-depth simulations. In this thesis, the equation of state of the jet fuel, JP-10, is incorporated into a multi-physics simulation code where JP-10 is exposed to high pressures, and decompressed into atmosphere. The simulation results are then compared to experiment results. Also, in a later chapter, the results from a separate numerical model is compared to the simulation results for added verification.

1.2 Aviation Fuels

The aviation fuel industry has come a long way since the increase in air travel since World War I. At the time, knock, carburetor icing, and vapor lock were issues that went undiagnosed. Now, fuel additives, better refining techniques, and strict fuel standards have made aviation fuel much more robust and efficient. There are several types of aviation fuels specific for certain applications. Aviation gasoline began as a general fuel for automobiles and aircraft before World War I, with little to no specifications. The performance of aviation gasoline
was very poor during this time. In 1918, the U.S. military wrote the first specification, and in later years, research was performed to reduce engine knock and other issues. During World War II, fuel standards were introduced so engines were designed with specific fuels. Today, the U.S. and much of the world uses grade 100LL aviation gasoline [5].

In 1948, the first turbine-powered flight was completed using British kerosine fuel. Since then, the U.S. used Jet A as the standard turbine fuel due to a lower freezing point. Non-U.S. countries use Jet A-1 that has an even lower freezing point. The first turbine fuel used by the United States military was called JP-1. Since only one percent of crude oil was separated into JP-1, alternative fuels were developed. Today, turbine fuels consist of three standard fuels, JP-4, JP-5, and JP-8, and two specialty fuels, JP-7 and JP-TS. Ramjet technology has led to the production of their own fuels which include RJ-4, RJ-5, and RJ-6. As of 2004, RJ-4 was the only active fuel in this category. Lastly, active grades for turbine missile engines include RJ-4 and JP-10. JP-9 was used before JP-10, but due to its high cost and inadequate low temperature properties, it was discontinued [5].

JP-10 is desired in many military applications such as cruise missiles and pulse detonation engines (PDE) for it’s low freezing point and high energy storage. PDEs are engines that generate thrust by detonating combustible propellant mixtures. These engines have the potential to revolutionize air travel due to their simple design, cycle efficiency, reliability, and ability to achieve super sonic speeds [7]. Since PDE’s require a hydrocarbon to detonate at high frequencies, extremely fast burn times are required. JP-10 is a good candidate for PDE’s due to it’s fast reaction rate and quick ignition delay time [8, 9]. However, more research and testing is required to achieve an operating engine.

1.3 Equation of State

In thermodynamics, the state of a material such as jet fuel is determined using what is called an equation of state (EOS). An EOS is a mathematical relationship that expresses intensive parameters such as temperature and pressure, in terms of independent extensive parameters such as internal energy or entropy [10]. For example, the internal energy of a material can be determined knowing the density and temperature, or \( E(\rho, T) \). In order for a material to be thermodynamically complete, all equations of state must be known, meaning that multiple intensive parameters are required.

There are many variations of EOS that describe certain materials such as high explosives, liquids, solids, and gasses. The most common and widely used EOS that defines ideal gases
is the ideal gas EOS developed from Boyle’s and Charles’ experiments [11]. Solids and liquids at high temperatures are typically modeled using the Mie-Grüneisen EOS, which is a function of the shock particle Hugoniot described in the following chapter, and the Grüneisen coefficient. The Grüneisen coefficient is characterized by the ratio of thermal pressure and thermal energy of an atomic lattice [12]. High explosives are often characterized by the Jones-Wilkins-Lee (JWL) equation of state that models the detonation product gases [13].

1.3.1 Experimental Methods

Equations of state for materials are typically determined via experiment. EOS are determined by varying one parameter, and seeing how the others change. For example, density of a fluid can be measured at constant pressure while allowing the temperature to change. This method is continued for other properties such as sound speed, viscosity, thermal conductivity, etc. However, these experiments are limited to relatively low pressures and temperatures. The most widely used method for determining equations of state at high pressures and temperatures involve shock waves. For example, the shock and resulting particle velocities in the desired material can be measured by various techniques. The shock-particle velocity relationship or Hugoniot of the material is used to formulate the Grüneisen EOS.

There are a couple of techniques to produce shock waves in solid and liquid materials that include high explosives (HE) and two-stage light gas guns. Conclusive high explosive induced shock wave studies originated by Walsh and Christian in 1955. They achieved planar shock wave pressure magnitudes from about 150-500 kilobars. They measured shock velocity and particle velocity using a high-speed sweep camera and a photographic record. The shock Hugoniots and P-v Hugoniots for aluminum, copper, and zinc were determined with an estimated error of 1-2% for pressure. They also calculated temperature and isotherms using thermodynamic identities and Hugoniot results [14]. Bancroft et al. in 1956 also used high explosives to generate shock waves in Armco iron and steel to determine the polymorphic transition to be about 0.13 Mbar. They incorporated time of arrival pins to measure shock velocity and pins to measure free surface motion. They determined the P-v Hugoniot for these materials using fundamental shock relations [15].

Two-stage light gas guns have been a more widely used technique in recent years. Lawrence Livermore National Laboratory uses a two-stage light gas gun to produce shock pressures from 20 GPa (200 kbar) for low-density materials up to 500 GPa (5 Mbar) for high-density materials. Shock temperature can reach tens of thousands of degrees (Kelvin), which makes applications for studying the earth’s core and mantle desireable. Also, the
initial states of the impactor and target material can be accurately measured because the impactor barely increases in temperature (1°C) during acceleration [16].

A two-stage light-gas gun operates in the following way. First, an energetic material such as black powder is burned allowing a piston to accelerate down a helium or hydrogen filled tube. The gas ahead of the piston increases pressure which opens a rupture valve and accelerates the projectile down the barrel [17]. The high velocity projectile strikes the desired material, creating a shock wave in the material. A flash x-ray measurement technique is used to measure the projectile velocity. A 20 g projectile can achieve 8 km/s. Shock waves are measured using shock arrival detectors such as self shorting coaxial pins or piezoelectric crystal pins fixed into the material and monitored using an oscilloscope.

In 2012, Robbins et al. performed shock compression measurements on fuel oil using a two-stage light gas gun. Particle velocity, shock velocity, and shock wave profiles were measured using embedded magnetic gauges. Magnetic particle velocity gauges are thin membranes that can be embedded in a sample and are used in non-metallic materials only. They operate using the principle of Faraday’s law of induction [18]. Projectile velocities were observed between 1.5 to 3.2 km/s. Shock pressures within the fuel oil ranged between 3-17 GPa. Also, their results showed good comparison against the Universal Liquid Hugoniot for hydrocarbons developed by Woolfolk et al. shown in Fig. 1.1 [1, 19].

Recent two-stage light gas gun experiments have been performed achieving extremely high pressures and shock velocities. In 2004, Knudson et al. from Sandia National Laboratory determined the pressure Hugoniot for cryogenic liquid deuterium using their Z accelerator. The Z accelerator uses a magnetic field to launch samples at hyper velocities. The electromag-
netic technology is similar to a railgun, except the Z accelerator uses much higher currents in a much shorter time period, and accelerates the flier plate to max velocity in millimeters instead of meters [20]. Pressures between 22-100 GPa were recorded. They launched a rectangular titanium flier plate (12 mm x 25 mm x 300 µm) up to 22 km/s and achieved shock velocities up to 28 km/s [21]. Velocity interferometry was used to measure plate acceleration and impact profiles. Velocity interferometry is a free surface motion measuring technique based on the doppler shift of laser frequencies [22].

1.4 Supersonic Liquid Jets

High velocity jets are produced from the decompression of a liquid, often produced from projectile impact, or high explosives within a nozzle. In this thesis, an explosively driven jet of JP-10 is produced for EOS purposes. Typically, high velocity liquid jets are studied by scientists interested in rain erosion on high velocity projectiles and jet aircraft, cleaning and cutting of materials, and mining applications. Rain drops can damage even the hardest materials at high rates of speed. This behavior has been experimentally proven by producing supersonic liquid jets and allowing them to contact fixed surfaces at specific distances. In 1958, Bowden and Brunton developed the first apparatus for efficiently producing supersonic flow of a liquid jet. The apparatus is quite simple, and works by compressing a small amount of liquid using a high-power air rifle. The projectile strikes an impact disk that rams the liquid through a nozzle. The nozzle outlet diameter was 1 mm. They imaged the jet formation using a six lens high-speed camera, and achieved jet velocities upwards of one km/s. They determined that an impact from a water jet (equivalent to the volume of a raindrop) can deform materials as hard as tungsten carbide [23].

More recently in 2006, Matthujak et al. imaged the jet formation of water, diesel fuel, kerosene, and gasoline at jet velocities up to one km/s using a high-speed camera and shadowgraph and interferometry techniques. They used a gravity driven two-stage light gas gun to accelerate a projectile into the liquid contained in a nozzle apparatus. The nozzle inlet diameter was 10.6 mm and the outlet diameter was 1 mm. The impact of the 300 m/s projectile on the liquid created pressures upwards of 12.4 GPa. A conical shock and several trailing oblique shock waves were imaged for each jet. Shadowgraphs of diesel fuel jets are shown in Fig. 1.2. It was shown that the geometry of the nozzle and the physical properties of each liquid has a large impact on the shape and velocity of each jet [2].

Earlier in 2001, Weeks et al. achieved much higher jet velocities via high explosives. They
designed an explosively driven water jet apparatus to achieve jet velocities up to 5 km/s. The nozzle apparatus is made from tempered steel, and up to 6 g of high explosives drive a piston against a liquid reservoir and nozzle. The nozzle dimensions were not discussed in this report, yet, they were able to accelerate 5 ml of liquid. They captured the jet and the jet’s contact against a piece of material using a high-speed framing camera shown in Fig. 1.3 [3].

Recent numerical results of a supersonic liquid jet were produced in 2015 by Majidi and Afshari. They developed and tested the first ghost fluid based numerical solver to model supersonic jets in a gaseous medium. A liquid with properties similar to diesel fuel was accelerated up to 450 m/s or Mach 3.36. Mach cones and oblique shocks were clearly evident in their simulations shown in Fig. 1.4, and showed how they changed as the jet velocity increased. They found that their simulations had good agreement with experimental results [4].
Figure 1.3: High-speed images of explosively driven water jet at 2.8 km/s at time delays of 6.7 μs per frame [3]
Figure 1.4: Numerical schlieren image of supersonic liquid jet at Mach 1.86 (250 m/s) [4]
Chapter 2

JP-10 Properties, Chemical Structure, and EOS

2.1 Physical and Chemical Properties

Jet Propellant 10 is a polycyclic alkane that is composed of mainly the exo isomer of tetrahydrodicyclopentadiene (tricyclo[5.2.1.0².⁶]decane, exo-THDCPD). A polycyclic alkane has a multi-ringed structure composed entirely of hydrogen and saturated carbon atoms and is shown in Fig. 2.1 for JP-10. The carbon to hydrogen ratio is 0.625 [24]. JP-10 is synthetically produced after hydrogenating endo-dicyclopentadiene, which yields a solid isomer, endo-tetrahydrodicyclopentadiene. This isomer is converted into exo-THDCPD (JP-10) by isomerization with sulfuric acid or aluminum chloride [25]. A gas chromatography-mass spectrometry analysis showed that JP-10 consists of major components exo-THDCPD (96.5% by mass), endo-THDCPD (2.5%), and adamantane (1.0%) [26]. Adamantane is a cycloalkane.

![Exo-Tetrahydrodi (Cyclopentadiene)](image)

Figure 2.1: Chemical structure of JP-10 [5]
and is the simplest diamondoid, which resembles a cubic diamond framework [25]. There were also several minor constituents found in JP-10 that include 2-methyl-bicyclo[3.2.1]octane, 2-ethyl-bicyclo[2.2.1]heptane, endo-2,2,3-trimethyl-bicyclo[2.2.1]heptane, cis-1-methyl-4-(1-methylethenyl)cyclohexane, and 2,6-dimethyl-bicyclo[3.2.1]octane [26].

The following physical properties of JP-10 were determined from the literature. JP-10 has a density of 0.932 g/cm$^3$, a kinematic viscosity of 2.97 mm$^2$/s, a speed of sound of 1405 m/s, and an adiabatic compressibility of 0.543 GPa$^{-1}$ at a temperature of 298 K and a pressure of 84 kPa [26]. The average molecular weight is 136 g/mol. JP-10 has a freezing point of about $-79^\circ$C. The heat of combustion is 44.5 MJ/kg [24]. JP-10 has an autoignition temperature of 245°C at standard pressure [5].

### 2.2 Equation of State for JP-10

The equation of state (EOS) for JP-10 was determined from experiment and literature by the National Institute of Standards and Technology (NIST) [26]. The EOS was defined explicitly in Helmholtz energy, which is the most widely used form to describe fluids and their properties. The Helmholtz potential or Helmholtz free energy, $F$, is defined as the partial Legendre transform of $U$ as a function of temperature, or more specifically,

$$F = U - TS$$

where $U$ is the internal energy, $T$ is temperature, and $S$ is entropy defined as $S = -\frac{\partial F}{\partial T}$. A Legendre transform is a mathematical technique that replaces extensive parameters with intensive parameters as independent variables [10]. The Helmholtz EOS contains only 10 terms because there isn’t enough experimental data to accurately generate a higher term EOS for JP-10. Usually, a high accuracy EOS contains between 20 to 50 fluid-specific terms, where density can be found to within 0.01% to 0.1% accuracy. For the purposes of this project, an EOS containing 10 terms is sufficient.

The derivation of the Helmholtz energy EOS was performed by methods used in [27]. The fundamental form of the Helmholtz energy can be expressed explicitly as

$$a(\rho, T) = a^0(\rho, T) + a^r(\rho, T),$$

where $a^0(\rho, T)$ is the ideal gas contribution and $a^r(\rho, T)$ is the real contribution of the Helmholtz energy. One can express the Helmholtz energy function in dimensionless form using the dimensionless density, $\delta = \rho/\rho_c$, and temperature, $\tau = T_c/T$, where $\rho_c$ and $T_c$...
are the critical density and pressure, respectively. The Helmholtz energy function can be re-written as

\[ a(\rho, T) = RT[\alpha^0(\delta, \tau) + \alpha^r(\delta, \tau)], \]  

where \( R \) is the ideal gas constant. The critical temperature, pressure, and density for JP-10 were experimentally found by Steele et al. [28]. The critical parameters were converted into the desired units for this study, along with the individual gas constant and molar mass of JP-10, and are listed in Table 2.1.

Table 2.1: Critical Properties for JP-10

<table>
<thead>
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<tr>
<td>( T_c )</td>
<td>698 K</td>
</tr>
<tr>
<td>( p_c )</td>
<td>3.733e-05 Mbar</td>
</tr>
<tr>
<td>( \rho_c )</td>
<td>0.2943 g/cm³</td>
</tr>
<tr>
<td>( R )</td>
<td>6.10326e-05 kJ/g K</td>
</tr>
<tr>
<td>( M )</td>
<td>136.23 g/mol</td>
</tr>
</tbody>
</table>

The ideal gas portion of the Helmholtz energy is given by

\[ \alpha^0(\delta, \tau) = a_1 + a_2 \tau + \ln \delta + (c_0 - 1) \ln \tau - \frac{c_1 T_c^{0.85}}{0.85(1.85)} \tau^{-0.85} - c_2 \ln[1 - \exp(-c_3 \tau/T_c)], \]  

where \( a_1 \) and \( a_2 \) are arbitrary coefficients chosen from the reference state for enthalpy and entropy, and \( c_0, c_1, c_2, \) and \( c_3 \) are specified constants. The arbitrary coefficients \( a_1 \) and \( a_2 \) were calculated via Stewart [29]

\[ a_1 = c_0 - 1 \ast R - 1 \ast s_0 + 1.176470588 \ast c_1 \ast \frac{T_0^{17/20}}{T_0} + c_0 \ln(T_0) - c_2 \ln(\exp(c_3/T_0) - 1) + c_2 c_3 \exp(c_3/T_0)/(T_0(\exp(c_3/T_0) - 1)) \]  

and

\[ a_2 = h_0 - 0.54054 c_1 T_0^{(37/20)} - c_2 c_3(\exp(c^3/T_0) - 1), \]  

where \( h_0 \) is the vaporization enthalpy of 49.1 kJ/mol determined by [30], \( s_0 \) is the initial entropy of 0.16468 kJ/mol K calculated by \( s_0 = h_0/T_0 \), and \( T_0 \) is the initial temperature given at 298.15 K. The values of the provided constants are \( c_0 = 3.3218, c_1 = 0.07975, c_2 = 27.6975, \) and \( c_3 = 1470 \) [26].
The real or residual fluid portion of the Helmholtz energy is given by

\[
\alpha^r(\delta, \tau) = n_1 \delta \tau^{0.2} + n_2 \delta \tau^{1.15} + n_3 \delta^2 \tau^{1.42} + n_4 \delta^2 \tau^{1.65} + n_5 \delta^4 \tau^2 + n_6 \delta^{3 \tau^2 \exp(-\delta)} + n_7 \delta^{3 \tau^{1.69} \exp(-\delta)} + n_8 \delta^{6 \tau^{0.95} \exp(-\delta)} + n_9 \delta^{6 \tau^{1.72} \exp(-\delta)} + n_{10} \delta^{6 \tau^{2.5} \exp(-\delta^2)},
\]

where \(n_1\) through \(n_{10}\) are coefficients determined by nonlinear fitting techniques for the equation of state. Table 2.2 shows the list of coefficients that are used in this portion of the EOS. Equations 2.4 and 2.7 are now useful in deriving the desired thermodynamic properties. The derivatives of the Helmholtz energy function produce the required thermodynamic properties needed for this study. For example, pressure is derived by

\[p = \frac{\partial a}{\partial v},\]

where \(v\) is specific volume [31]. The internal energy is derived from

\[U = a(\rho, T) + TS,\]

where entropy is determined by the function \(S = \frac{\partial a}{\partial T}\). Also, several thermodynamic properties were derived by Lemmon et al. [27] and shown in Bruno et al. [26]. Pressure, energy per unit mass, and sound speed as functions of dimensionless density and temperature were given as

\[
P(\delta, \tau) = \frac{RT_c \delta \rho_c}{\tau} \left[ 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau \right],\]

\[
e(\delta, \tau) = \frac{RT_c}{M} \left[ \left( \frac{\partial \alpha^r}{\partial \tau} \right)_\delta + \left( \frac{\partial \alpha^r}{\partial \tau} \right)_\delta \right],\]

(2.8)

(2.9)
\[
\frac{w^2M}{RT} = 1 + 2\delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau + \delta^2 \left( \frac{\partial^2 \alpha^r}{\partial \delta^2} \right)_\tau - \frac{1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau - \delta \frac{\partial^2 \alpha^r}{\partial \delta \partial \tau}}{\tau^2 \left[ \left( \frac{\partial^2 \alpha^0}{\partial \tau^2} \right)_\delta + \left( \frac{\partial^2 \alpha^r}{\partial \tau^2} \right)_\delta \right]}^2,
\]

(2.10)

where the partial derivatives of \(\alpha^0\) and \(\alpha^r\) with respect to \(\delta\) and \(\tau\) can be calculated. The accuracy of this EOS was determined by Bruno et al. [26]. Density is within 0.04\% of the experimental measurements. However, the experimental measurements were not conducted above atmospheric pressure, above a temperature of 400 K, or in the vapor phase. The density for saturated liquid or vapor points were fit from seven data points from Steele et al. [28]. The vapor pressure measurements were lacking for their (Bruno et al.) work, and the single vapor pressure measured was fit to less than 0.1\%. The equation for the ideal gas heat capacity (not shown in this thesis) is accurate to less than 0.4\% of the data gathered by [32]. The equation for the speed of sound was accurate to less than 0.04\% of the experiment measurements.

The pressure, internal energy, and sound speed from Eqs. 2.8-2.10 were plotted as functions of specific volume and temperature to form 3D surfaces. These 3D surfaces describe the Helmholtz EOS for JP-10 using units often used in the energetic materials industry (Mbar, \(\mu\)s, cm). Figure 2.2 shows the surface plot of pressure ranging from 0 to 0.2 Mbar. At larger specific volumes, the pressure flattens out and approaches zero. Temperature does not have a large effect on pressure at high volumes. As the specific volume approaches 0.55 \(cm^3/g\), the pressure increases non-linearly to upwards of 0.20 Mbar. Internal energy is shown in Fig. 2.3 with the same range of volumes and temperatures. The internal energy varies from -0.80 \(kJ/g\), to -0.745 \(kJ/g\) in this plot, and one can see that temperature has a large effect on internal energy, ranging from 200 K to 1500 K. At high temperatures and low volumes, the internal energy is at it’s highest. The surface plot of sound speed is shown in Fig. 2.4. The sound speed is highest at low volumes and temperatures, and lowest at high temperatures and volumes.
Figure 2.2: $P(v,T)$ surface plot of Helmholtz EOS of JP-10

Figure 2.3: $e(v,T)$ surface plot of Helmholtz EOS of JP-10
2.3 Shock Relations

A normal shock wave that moves within a fluid such as JP-10 can be analyzed. A normal shock wave can be treated as a jump condition, where the thermodynamic states before and after a shock are calculated. These states can be calculated using the Rankine-Hugoniot (R-H) jump relations that are derived from the fluid conservation equations. The conservation of mass, also known as the continuity equation, relates the mass exchange in and out of a system. The conservation of momentum, derived using Newton’s second law, states that a fluid’s momentum is equal to the net external forces acting on the fluid. The conservation of energy, derived from the first law of thermodynamics, states that the change in internal energy of a fluid is equal to the sum of the total work done on the fluid and any heat that was added \[33, 34, 35\]. The conservation of mass, momentum, and energy, assuming inviscid flow, are shown in conservative form as

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho \mathbf{v}) = 0,
\]

(2.11)

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \mathbf{v} \frac{\partial}{\partial x} (\rho \mathbf{v}) + \frac{\partial p}{\partial x} = \rho \mathbf{F},
\]

(2.12)

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \rho e \right) + \frac{\partial}{\partial x} \left[ \left( \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \rho e + p \right) \mathbf{v} \right] = \rho \mathbf{F} \mathbf{v},
\]

(2.13)
where $F$ is the external force per unit mass acting on the fluid. From here, one can simplify the conservation equations to produce the desired Rankine-Hugoniot equations in the Lagrangian coordinate frame. The R-H jump equations are shown as

\begin{align}
\text{mass:} & \quad \frac{\rho_1}{\rho_0} = \frac{U_s - U_{p0}}{U_s - U_{p1}} = \frac{v_0}{v_1}, \quad (2.14) \\
\text{momentum:} & \quad P_1 - P_0 = \frac{1}{v_0} (U_{p1} - U_{p0}) (U_s - U_{p0}), \quad (2.15) \\
\text{energy:} & \quad e_1 - e_0 = \frac{v_0 (P_1 U_{p1} - P_0 U_{p0})}{U_s - U_{p0}} - \frac{1}{2} (U_{p1}^2 - U_{p0}^2), \quad (2.16)
\end{align}

where $U_s$ is the shock velocity, $U_p$ is the particle velocity, and the subscripts 0 and 1 represent the states in front and behind the shock front, respectively [36]. One can solve these equations for pressure as a function of specific volume to obtain the desired relationship called the $P - \nu$ Hugoniot equation. The $P - \nu$ Hugoniot describes the locus of all the possible equilibrium states that a material can exist. However, in order to solve the Hugoniot equation, a relationship between shock velocity and particle velocity is needed. Often called the $U_s - U_p$ relationship, this linear equation is shown as

$$U_s = C_0 + s U_p,$$  \hspace{1cm} (2.17)

where $C_0$ is considered the bulk sound speed, but is really a non-physical term that describes the y-axis intercept, and $s$ is the slope of the line [36]. The values for $C_0$ and $s$ are experimentally determined by exposing a material to many shock wave strengths, and measuring the associated particle velocities. This relationship is then linearly fit to the $U_s - U_p$ equation. For this project, the experimental values of $C_0$ and $s$ for JP-10 are unknown, so the $U_s - U_p$ relationship is determined via the Helmholtz EOS and the R-H equations, assuming that $U_{p0}=0$, $\rho_0=0.931$ g/cm$^3$, $P_0=1$e-06 Mbar, and $T_0=298.15$ K. Equations 2.8 and 2.9 are substituted into Eqs. 2.14 and 2.15. By changing values of $\tau$ from 0.4 to 2.34, the system of equations were solved for $\rho_1$, $U_s$, and $U_p$ producing a table of values. The results were linearly fit to Eq. 2.17 to produce the desired $U_s - U_p$ relationship for JP-10. This relationship for JP-10 was plotted and is shown in Fig. 2.5, where $C_0$ and $s$ are 0.156 cm/µs and 1.617, respectively.
The $P - v$ Hugoniot can be solved by substituting the $U_s - U_p$ equation into Eqns. 2.14-2.15 and assuming $P_0 = U_{p0} = 0$. The $P - v$ Hugoniot is only a function of $C_0$, $v$, and $s$, and is shown as

$$P = C_0^2(v_0 - v)[v_0 - s(v_0 - v)]^{-2},$$

where $v_0$ is the initial unshocked specific volume of the material [36]. The $P - v$ Hugoniot can also be a close estimation of the isentrope of the material. The isentrope and $P - v$ Hugoniot are not exactly equal, but for engineering purposes, they are considered a close approximation. Since the $P - v$ Hugoniot represents all possible states in front and behind of a shock front, they can be connected by what is known as a Raleigh line. The equation for the Raleigh line is developed by manipulating the R-H equations and assuming $U_{p0} = 0$. The Raleigh line is a function of shock velocity (not particle velocity) and is shown as

$$P_1 - P_0 = \frac{U_s^2}{v_0} - \frac{U_s^2}{v_1^2}v_1,$$

where the slope of the line is $-U^2/v_0^2$. The Raleigh line is a very important addition to the $P - v$ Hugoniot because it allows one to calculate the final states of the shock wave knowing the initial state and the shock velocity. Also, one can calculate the shock velocity if the initial and final $P - v$ states are known. The $P - v$ Hugoniot and Raleigh line for JP-10 using the Helmholtz EOS can be seen in Fig. 2.6. The Raleigh line was plotted at an arbitrary shock velocity of 0.288 cm/µs from an initial specific volume of 1.07 cm$^3$/g and a pressure of 1e-06 Mbar. One can see from this example that the shock front increases the pressure of JP-10 to
above 0.02 Mbar at a specific volume of 0.77 cm$^3$/g. If the shock velocity were greater than in this example, then the slope of the Raleigh line would decrease, and the final pressure would be higher. The $P - v$ Hugoniot and Raleigh line not only describe the initial and final states of a shock, but also the specific kinetic energy of the material behind the shock front. The increase in kinetic energy is determined by calculating the area under the Raleigh line between the intersecting points at $P_0$ and $P_1$. Also, one can determine the change in specific internal energy by calculating the total area under the Raleigh line between $P_1$ and $P = 0$ at the intersection with the $P - v$ Hugoniot.
Chapter 3

Experiment

3.1 Experiment Setup

3.1.1 Nozzle Assembly

I performed an experiment with Prof. Nick Glumac at the University of Illinois at Urbana-Champaign. The goal of this experiment is to determine the effects of rapidly decompressing JP-10 by capturing high-speed images of the formed jet and measuring shock velocity within the JP-10 contained in the nozzle. This experiment was performed at standard temperature and pressure (1 atmosphere). The nozzle apparatus is composed of several parts and is shown in Fig. 3.1. A total of 5 nozzles were machined from 303 Stainless Steel (SS) and have the dimensions shown in Appendix A. Typically, 304 SS is used in the laboratory setting, however, since 303 SS is much easier/quicker to machine and has similar mechanical properties as 304 SS, 303 SS was used instead. All dimensions of the nozzle were the same as in the ALE3D simulations, except for the diameter of the acrylic (Lucite) mitigator and the baseplate. This time, the mitigator has the same diameter as the nozzle inlet (2.54 cm or 1 inch). The acrylic disk acts as a mitigator that separates the HE from the liquid. The edge was coated with thick grease to prevent any liquid from leaking during assembly. The baseplate is a square piece of steel with a length of 10.16 cm (4 inches).

Using epoxy, we attached two piezoelectric pins from the top of the nozzle into the nozzle inlet containing the liquid. The piezoelectric pins are used for measuring the time of arrival (TOA) of the leading shock produced from detonating the high explosives (HE). These pins are manufactured by Dynasen, Inc. and are capable of measuring TOA from pressures between a few psi up to 300 kbar with a 10 nanosecond response time and a maximum output voltage of about 600 volts [37]. The pins are 0.064 inch in diameter and 2 inches in
The HE used in the experiment was Primasheet-1000 which is similar to Detasheet-C used in the simulations. We cut thin cylinders of HE having a diameter of one inch, and a thickness of 0.0787 inch (2 mm). We varied the mass of HE by adding layers to the nozzle. A single layer consisted of approximately 1.5 grams of HE. The layer or layers of HE were placed between the steel baseplate and the PMMA disk within the nozzle. The low carbon steel baseplate has the dimensions 4” x 4” x 1/2”. Four 1/4”-20 x 7/8” black oxide alloy steel screws fixed the nozzle to the baseplate. Once the nozzle was secure against the baseplate, the liquid was injected via syringe through the nozzle outlet. The liquid was injected until the surface was flush with the nozzle outlet. The stand is necessary to elevate the nozzle assembly to the appropriate viewing height. A RISI RP-501 Economy EBW detonator initiates the main HE through the center hole of the baseplate [38]. The detonator is 0.295 inch in diameter and 0.825 inch in length. Figures 3.2 and 3.3 show the finished nozzle assembly resting on top of a steel stand.
Figure 3.2: Nozzle assembly ready for shooting
Figure 3.3: Nozzle assembly with stand
3.1.2 Instrumentation and Schematic

The experiment consisted of several components and measurement instruments that can be seen in Fig. 3.4. The nozzle assembly was placed in a 4 x 4 x 4 ft steel blast chamber and attached to a stand to elevate the nozzle to the appropriate viewing height. The experiment begins with the pulse generator that simultaneously sends an electrical signal to the framing camera, firing system, oscilloscope, and the light source. This initial pulse activates each device which is synchronized to operate at specific times. The 9520 Digital Delay Pulse Generator is manufactured by Quantum Composers and offers up to eight independent channel outputs with a resolution of 250 ps [39].

When triggered by the pulse generator, the firing system sends a high voltage/amp pulse to the detonator that initiates the high explosives. The Teledyne RISI (Reynolds Industries Systems Incorporated) FS-43 Firing System consists of a control unit and firing module [40]. The separate firing module allows long distance and remote firings if necessary. The firing system operates on standard 110 volt AC input and produces a 4000 volt pulse with 1500 ampere peak current into a low resistance load (8 joules).

The framing camera captures high-speed images of the jetting event through acrylic windows along the blast chamber walls. Manufactured by PCO, the HSFC Pro image intensifier (MCP) 12 bit high-speed framing camera has the ability to capture four full frame resolution images with one nano second interframing time [41]. Four high resolution CCD image sensors (1280 x 1024 pixel) capture the event and is controlled by the HSFC Pro camware software on a personal computer. Because the interframing time is so low, a large amount of light is necessary to record bright and clear images. Therefore, a light source is required and is placed directly across from the framing camera. A Photogenic PowerLight 2500DR is used to provide the extra light for the camera [42]. This camera is capable of producing up to 1000 watt-seconds of flash power with three seconds of recycle time at full power.

A Pico Technology PicoScope 3424 PC Oscilloscope in combination with PicoScope 6 PC Oscilloscope Software is used to gather and record the output voltages from the piezoelectric TOA pins [43]. The 12 bit resolution oscilloscope has a maximum sampling rate of 5 MS/s while using all four BNC channels and an accuracy of 1 % of the voltage (50 ppm time). The voltage range for this oscilloscope is ±20 mV to ±20 V. Recalling that the output voltage of the piezoelectric TOA pins can potentially reach 600 volts, attenuators are placed in series between the TOA pins and the oscilloscope to reduce the voltage to a safe level below 20 volts. A JFW Industries 50F-030 BNC Fixed Attenuator is placed in series along each of the two BNC cables connecting the oscilloscope to the piezoelectric pins [44]. The attenuators
have a 30 decibel attenuation value that reduces the output voltage from 600 to 18.75 volts.

Figure 3.4: Experiment instrumentation and setup (not to scale)

### 3.2 Experiment Results

A total of five shots were performed using all five nozzles containing varying masses of HE and liquid. Four nozzle experiments were performed with JP-10, and one with water as a control because water has a well established EOS. Tables 3.1 and 3.2 show the tabulated results of the five nozzles using JP-10 and water, and Figs. 3.5 - 3.29 show the high-speed images of the jet events. Each set of high-speed images for each nozzle was captured using different time delays, except for Nozzles 1 and 2. These nozzles were captured at the same time delays for comparison purposes between water and JP-10 using similar amounts of HE.

All nozzles except Nozzle 5 were successful in providing clear images of the emerging jet from the nozzle. Nozzle 5 failed catastrophically due to excessive pressure from too much HE. Although each nozzle ultimately failed at later times after detonation, Nozzle 5 failed much more significantly as shown in Fig. 3.30. The stainless steel nozzle fractured in
several places including the diverging section of the nozzle. The other 4 nozzles with less HE experienced less damage similar to Nozzle 3. The nozzle split into four segments initiating along the threaded screw holes, up to the nozzle outlet. The diverging section of the nozzle was intact unlike Nozzle 5. Because the diverging section of Nozzle 5 fractured, the HE product gasses were allowed to escape around the fluid jet. As you can see in Fig. 3.28, the product gasses are already escaping through the nozzle exit and disrupt the view of the JP-10 jet. Therefore, I was unable to measure the jet velocity for Nozzle 5, and I believe the shock velocity was also inaccurate.

As expected, both the shock velocity and jet velocity increased as the mass of HE increased. However, during Nozzle 5, the shock velocity was actually lower than Nozzle 4, and the cause might be related to the premature failure of the nozzle mentioned previously. The jet velocities for all shots were greater than the shock velocities. This phenomena is often seen in shaped charges where the high velocity slug of material exceeds the post detonation shock velocity [45].

### Table 3.1: Experiment Results for Water

<table>
<thead>
<tr>
<th>Nozzle Number</th>
<th>Mass of HE [g]</th>
<th>Mass of Water [g]</th>
<th>Shock Velocity ±0.001 [cm/µs]</th>
<th>Jet Velocity ±0.001 [cm/µs]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.49</td>
<td>10.58</td>
<td>0.248</td>
<td>0.287</td>
</tr>
</tbody>
</table>

### Table 3.2: Experiment Results for JP-10

<table>
<thead>
<tr>
<th>Nozzle Number</th>
<th>Mass of HE [g]</th>
<th>Mass of JP-10 [g]</th>
<th>Shock Velocity ±0.001 [cm/µs]</th>
<th>Jet Velocity ±0.001 [cm/µs]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.51</td>
<td>9.75</td>
<td>0.288</td>
<td>0.344</td>
</tr>
<tr>
<td>3</td>
<td>1.50</td>
<td>9.90</td>
<td>n/a*</td>
<td>0.365</td>
</tr>
<tr>
<td>4</td>
<td>2.99</td>
<td>8.96</td>
<td>0.321</td>
<td>0.458</td>
</tr>
<tr>
<td>5</td>
<td>4.41</td>
<td>7.90</td>
<td>0.312**</td>
<td>n/a</td>
</tr>
</tbody>
</table>

*Malfunctioned piezoelectric pin*  
**Inaccurate results from catastrophically failed nozzle**

The basic shape of the JP-10 and water jets are all similar to one another. The jet can be characterized as two parts: the bulged and stretched sections. The bulged section of the
jet is the thickest portion that trails the stretched part of the jet. The stretched section is much thinner and often has a rounded or "flower" shape at the leading jet tip. This decrease in cross sectional area is due to a stretching occurrence caused from a velocity gradient. The velocity is greatest near the jet tip, and decreases towards the bulged region of the jet. The stretched region also appears to have a smooth defined surface while the bulged section appears to be more turbulent and rough. Side-by-side high-speed images are provided in Appendix B.

Figure 3.5: High-speed Image of Nozzle 1, Frame 1, with 1.49 g HE and 10.58 g water
Figure 3.6: High-speed Image of Nozzle 1, Frame 2, with 1.49 g HE and 10.58 g water

Figure 3.7: High-speed Image of Nozzle 1, Frame 3, with 1.49 g HE and 10.58 g water
Figure 3.8: High-speed Image of Nozzle 1, Frame 4, with 1.49 g HE and 10.58 g water

Figure 3.9: High-speed Image of Nozzle 1, Frame 5, with 1.49 g HE and 10.58 g water
Figure 3.10: High-speed Image of Nozzle 2, Frame 1, with 1.51 g HE and 9.75 g JP-10

Figure 3.11: High-speed Image of Nozzle 2, Frame 2, with 1.51 g HE and 9.75 g JP-10
Figure 3.12: High-speed Image of Nozzle 2, Frame 3, with 1.51 g HE and 9.75 g JP-10

Figure 3.13: High-speed Image of Nozzle 2, Frame 4, with 1.51 g HE and 9.75 g JP-10
Figure 3.14: High-speed Image of Nozzle 2, Frame 5, with 1.51 g HE and 9.75 g JP-10
Figure 3.15: High-speed Image of Nozzle 3, Frame 1, with 1.50 g HE and 9.90 g JP-10

Figure 3.16: High-speed Image of Nozzle 3, Frame 2, with 1.50 g HE and 9.90 g JP-10
Figure 3.17: High-speed Image of Nozzle 3, Frame 3, with 1.50 g HE and 9.90 g JP-10

Figure 3.18: High-speed Image of Nozzle 3, Frame 4, with 1.50 g HE and 9.90 g JP-10
Figure 3.19: High-speed Image of Nozzle 3, Frame 5, with 1.50 g HE and 9.90 g JP-10
Figure 3.20: High-speed Image of Nozzle 4, Frame 1, with 2.99 g HE and 8.96 g JP-10

Figure 3.21: High-speed Image of Nozzle 4, Frame 2, with 2.99 g HE and 8.96 g JP-10
Figure 3.22: High-speed Image of Nozzle 4, Frame 3, with 2.99 g HE and 8.96 g JP-10

Figure 3.23: High-speed Image of Nozzle 4, Frame 4, with 2.99 g HE and 8.96 g JP-10
Figure 3.24: High-speed Image of Nozzle 4, Frame 5, with 2.99 g HE and 8.96 g JP-10
Figure 3.25: High-speed Image of Nozzle 5, Frame 1, with 4.41 g HE and 7.90 g JP-10

Figure 3.26: High-speed Image of Nozzle 5, Frame 2, with 4.41 g HE and 7.90 g JP-10
Figure 3.27: High-speed Image of Nozzle 5, Frame 3, with 4.41 g HE and 7.90 g JP-10

Figure 3.28: High-speed Image of Nozzle 5, Frame 4, with 4.41 g HE and 7.90 g JP-10
Figure 3.29: High-speed Image of Nozzle 5, Frame 5, with 4.41 g HE and 7.90 g JP-10

$t = 61 \, \mu s$
Figure 3.30: Pieces obtained from overly fractured Nozzle 5 (Top) and ideally fractured Nozzle 3 including the PMMA mitigator (Bottom)
A side-by-side comparison of the water filled nozzle and the JP-10 filled nozzle is shown in Figs. 3.31 - 3.34. The shapes of the jets are noticeably different. First, the water jet is much more rough throughout the bulged and stretched portions. Also, the jet is thicker and the geometry is less defined. The velocity of the water jet is $0.057 \text{ cm/µs}$ less than the JP-10 jet. The shock velocity within water is $0.04 \text{ cm/µs}$ slower as well. This comparison shows that the properties and EOS of water is different from JP-10, and is a good control material.

Figure 3.31: Water (left) and JP-10 (right) side-by-side comparison using $\sim 1.5 \text{ g HE}$
Figure 3.32: Water (left) and JP-10 (right) side-by-side comparison using $\sim 1.5 \text{ g HE}$

Figure 3.33: Water (left) and JP-10 (right) side-by-side comparison using $\sim 1.5 \text{ g HE}$
Figure 3.34: Water (left) and JP-10 (right) side-by-side comparison using \( \sim 1.5 \) g HE
Chapter 4

Baseline Simulation

4.1 ALE3D Overview

Four baseline simulations were performed in two-dimensions using the software ALE3D to develop an in-depth understanding of the nozzle event, and to compare the results to the experiment. Computational simulations offer a cost efficient alternative to experiments and provide scientists/engineers with the ability to quickly modify and test current experiment designs. ALE3D is a powerful multi-physics numerical simulation software tool developed by Lawrence Livermore National Laboratory (LLNL). ALE3D utilizes arbitrary Lagrangian-Eularian (ALE) techniques to simulate complex engineering and physics problems in two-dimensional or three-dimensional space. A hybrid finite element and finite volume formulation is used to model flows and other processes. There are many applications for ALE3D including detonation, deflagration, convective burn, fracture, fragmentation, heat transfer, incompressible flow, magneto-hydrodynamics, and many more [46]. ALE3D is a tedious program and requires a lot of trial and error, thus, over 30 simulations were performed to reach the final result.

4.2 Simulation Setup

4.2.1 Materials and Dimensions

The ALE3D simulations were performed axisymmetrically along the x-axis (labelled as Length) to reduce the computational time and file size. The entire domain of the simulation can be seen in Fig. 4.1, which includes a color representation of the geometries. The materials and their representative colors are shown in Table 4.1. A closer view of the nozzle
components can be seen in Fig. 4.2. One should note that the experiment was conducted vertically, whereas the simulations were conducted horizontally. Since the material velocities are so high, and time delays are so fast, gravitational forces are disregarded.

All four simulations have the same geometry and dimensions, except for the amount of HE and liquid. The first simulation was performed with water because water has a well established EOS, and is a good control. The remaining three simulations were performed with JP-10 using three increasing amounts of high explosive. The simulation results were visualized using an open source, interactive, visualization, and analysis tool called VisIt that was developed by the Department of Energy [47]. One should take note that both the stainless steel nozzle and the steel baseplate are shown in red. These two materials are joined at the top of the baseplate. One can also see in this figure that there is a slight gap between the lucite mitigator and the stainless steel nozzle inner wall. The purpose for this gap is to reduce friction because when two or more materials touch one another, ALE3D defaults to fusing those materials (like the baseplate and nozzle). To accommodate this, ALE3D offers a "slide surface" option that allows the user to modify friction effects between two or more touching surfaces. The user can set friction to zero if necessary. However, this option can complicate the mesh process and is more time consuming, so no slide surfaces were used in this thesis.

The following dimensions for the nozzle and its components are expressed next. The baseplate thickness is 1.27 cm (0.5 inch), and the diameter is 8 cm (3.15 inch). The detonator hole within the baseplate has a diameter of 0.749 cm (0.295 inch). The nozzle angle is 45° from the centerline (x-axis), the nozzle inlet diameter is 2.54 cm (1 inch), and the outlet diameter is 0.476 cm (3/16 inch). The nozzle outer diameter is 5.08 cm (2 inches), and the total height is 3.73 cm (1.47 inch). The acrylic (Lucite) disk acts as a mitigator that separates the HE from the liquid. The mitigator has a diameter of 0.98 inch (2.49 cm) and a thickness of 0.476 cm (3/16 inch). The thickness of the main HE depends on the mass desired. Detasheet-C, with a diameter of 2.54 cm (1 inch) and a thickness of 0.2 cm, has a mass of roughly 1.50 g. Simulations were performed using Detasheet-C thicknesses of 0.2, 0.4, and 0.6 cm.

4.2.2 Mesh and Boundary Conditions

In order to avoid mesh errors such as small volume fractions and mesh entanglement, a uniform square mesh was used. A single mesh was produced for all materials with a total of 112,500 elements and a characteristic element size of 0.0267 cm. Typically, a finer mesh is
Figure 4.1: Entire domain of ALE3D initial geometry shown in Visit at $t=0 \, \mu s$

Figure 4.2: Close-up of the nozzle components at $t=0 \, \mu s$

Table 4.1: ALE3D Material Components

<table>
<thead>
<tr>
<th>Material</th>
<th>Color</th>
<th>Model Part</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel (Vascomax 250)</td>
<td>Red</td>
<td>Baseplate</td>
</tr>
<tr>
<td>Stainless Steel (304)</td>
<td>Red</td>
<td>Nozzle</td>
</tr>
<tr>
<td>PETN</td>
<td>Light Grey</td>
<td>Detonator HE</td>
</tr>
<tr>
<td>PBX9407</td>
<td>Light Blue</td>
<td>Detonator HE</td>
</tr>
<tr>
<td>Detaasheet-C</td>
<td>Blue</td>
<td>Main HE</td>
</tr>
<tr>
<td>Lucite</td>
<td>Orange</td>
<td>Mitigator</td>
</tr>
<tr>
<td>JP-10/water</td>
<td>Green</td>
<td>Liquid</td>
</tr>
<tr>
<td>Air</td>
<td>Salmon</td>
<td>Atmosphere</td>
</tr>
</tbody>
</table>
desired to reduce the viscous dominating forces of jetting materials. However, the simulations failed prematurely using a finer mesh, even after making dozens of modifications to the simulation settings. Later attempts to reduce the mesh size were discontinued.

Since the simulations were performed using 2D axisymmetry about the x-axis, the elements along the centerline at y=0 were treated as axisymmetric elements. The elements along x=0, x=xmax, and y=ymax were treated as non-reflecting boundary conditions so that any high velocity material can escape the domain freely like in the real experiment. In the experiment, the baseplate and nozzle assembly rest on hex nuts attached on threaded rods. Therefore, a fixed square boundary condition was applied to the steel baseplate from the outer edge to 0.5 inches toward the centerline to replicate a fixed joint. Also, as mentioned earlier in this section, the nozzle was fused to the baseplate along the bottom of the nozzle. However, in the experiment, the nozzle was fixed to the baseplate via screws. Since the simulations are axisymmetric, it is not possible to add screws to the assembly. The affects of this will be discussed in a later chapter.

4.2.3 Material Parameters

The material parameters and associated EOS’s used in the ALE3D simulations are shown in Table 4.2. The properties for the HE materials PETN and PBX-9407 were determined by Teledyne that are used in their RP-501 detonators. The RP-501 detonator was used in the upcoming experiment and contained about 149 mg of PETN pressed to about 50% of the theoretical maximum density, or TMD (0.88 g/cm$^3$), and 227 mg of PBX-9407 pressed to 90% TMD (1.6 g/cm$^3$) [48]. Parameters for Detasheet-C were used instead of Primasheet-1000 from the experiment because Detasheet-C has a similar mixture of explosives, and the parameters are well documented [36].

4.2.4 Grüneisen EOS

The Grüneisen EOS is used to model non-reactive solids and some liquids and is given by [49]

$$P = \frac{\rho_0 c^2}{\mu} \left[ 1 + \left( 1 - \frac{\gamma_0}{2} \right) \frac{\mu}{2} - \frac{\mu^2}{2} \right] \left[ 1 - (S_1 - 1)\mu - \frac{\mu^2}{(\mu + 1)} - \frac{\mu^3}{(\mu + 1)^2} \right]^2 + (\gamma_0 + a\mu)e. \quad (4.1)$$

The Grüneisen EOS is expressed in terms of the parameters $c, S_1, S_2, S_3, \gamma_0,$ and $a$. The parameter $c$ is the intercept of the $U_s - U_p$ curve, (shock Hugoniot), and $S_1, S_2,$ and $S_3$ are...
<table>
<thead>
<tr>
<th>Material</th>
<th>Density ([\text{g/cm}^3])</th>
<th>Initial Energy [kJ]</th>
<th>EOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel (Vascomax 250)</td>
<td>8.129</td>
<td>0</td>
<td>Grüneisen</td>
</tr>
<tr>
<td>Stainless Steel (304)</td>
<td>7.9</td>
<td>0</td>
<td>Grüneisen</td>
</tr>
<tr>
<td>PETN</td>
<td>0.88</td>
<td>0.0502</td>
<td>JWL</td>
</tr>
<tr>
<td>PBX-9407</td>
<td>1.6</td>
<td>0.09</td>
<td>JWL</td>
</tr>
<tr>
<td>Detasheet-C</td>
<td>1.48</td>
<td>0.062</td>
<td>JWL</td>
</tr>
<tr>
<td>Lucite</td>
<td>1.182</td>
<td>0</td>
<td>Grüneisen</td>
</tr>
<tr>
<td>JP-10</td>
<td>0.931</td>
<td>0</td>
<td>Grüneisen</td>
</tr>
<tr>
<td>Water</td>
<td>1.0</td>
<td>0</td>
<td>Grüneisen</td>
</tr>
<tr>
<td>Air</td>
<td>0.0013</td>
<td>2.5e-06</td>
<td>Gamma Law</td>
</tr>
</tbody>
</table>

The coefficients of the slope of the \(U_s - U_p\) curve. The parameter \(\gamma_0\) is the Grüneisen gamma, and \(a\) is the first order volume correction to \(\gamma\). The dimensionless parameter \(\mu\) is a function of density and was given as \(\mu = \rho/\rho_0 - 1\). The Hugoniot \((U_s - U_p)\) relation solved within ALE3D is expressed by the cubic equation

\[
\frac{c_0}{U_s} = 1 - S_1 \left( \frac{U_p}{U_s} \right) - S_2 \left( \frac{U_p}{U_s} \right)^2 - S_3 \left( \frac{U_p}{U_s} \right)^3.
\] (4.2)

Multiple steps were performed to fit the Helmholtz EOS of JP-10 to the Grüneisen EOS used in ALE3D. First, the R-H equations (Eqs. 2.14 - 2.16) were manipulated and solved for \(U_p/U_s\) and \(U_s\) in a similar process to that of the Hugoniot of JP-10 shown in Fig. 2.5. The tabulated solution was then fit to Eq. 4.2 using a built in nonlinear fitting method from Wolfram Mathematica software. The coefficients \(c_0\), \(S_1\), \(S_2\), and \(S_3\) were determined from this fit, and prove to be a very close match shown in Fig. 4.3. The Grüneisen gamma was found using the fundamental equation

\[
\gamma = v \left( \frac{\partial P}{\partial E} \right)_v = \frac{v \left( \frac{\partial P}{\partial T} \right)_v}{\left( \frac{\partial E}{\partial T} \right)_v},
\] (4.3)

where the derivatives are calculated from the Helmholtz EOS of JP-10 [51]. Lastly, \(a\) was set to zero because there is no volume correction to \(\gamma\). Table 4.3 shows all of the Grüneisen EOS coefficients for the applicable materials.
Figure 4.3: Non-linear fit of $U_s-U_p$ Hugoniot for JP-10

Table 4.3: Material Grüneisen EOS Coefficients [49, 52]

<table>
<thead>
<tr>
<th>Material</th>
<th>$c$</th>
<th>$S_1$</th>
<th>$S_2$</th>
<th>$S_3$</th>
<th>$\gamma_0$</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel (Vascomax 250)</td>
<td>0.398</td>
<td>1.58</td>
<td>0</td>
<td>0</td>
<td>1.6</td>
<td>0.5</td>
</tr>
<tr>
<td>Stainless Steel (304)</td>
<td>0.457</td>
<td>1.49</td>
<td>0</td>
<td>0</td>
<td>1.93</td>
<td>0.5</td>
</tr>
<tr>
<td>Lucite</td>
<td>0.218</td>
<td>2.088</td>
<td>-1.124</td>
<td>0</td>
<td>0.85</td>
<td>0</td>
</tr>
<tr>
<td>JP-10</td>
<td>0.1394</td>
<td>2.46</td>
<td>-2.296</td>
<td>1.014</td>
<td>1.067</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>0.148</td>
<td>2.56</td>
<td>-1.986</td>
<td>0.227</td>
<td>0.5</td>
<td>0</td>
</tr>
</tbody>
</table>

4.2.5 Gamma Law Gas EOS

Gasses are modeled using the Gamma Law Gas EOS shown as

$$P = (\gamma - 1) \frac{\rho}{\rho_0}e,$$  \hspace{1cm} (4.4)

where $\gamma$ is the ratio of specific heats of the gas, and $e$ is the internal energy per unit volume [49]. The value for air can be seen in Table 4.4.
Table 4.4: Material Gamma Law EOS Coefficient

<table>
<thead>
<tr>
<th>Material</th>
<th>$(\gamma - 1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.4</td>
</tr>
</tbody>
</table>

4.2.6 JWL High Explosive EOS

The Jones Wilkins Lee (JWL) equation of state is used to model the detonation products of high explosives. The JWL EOS is shown as

$$P = A \left( 1 - \frac{w}{R_1 v} \right) \exp(-R_1 v) + B \left( 1 - \frac{w}{R_2 v} \right) \exp(-R_2 v) + \frac{w}{v} e, \quad (4.5)$$

where $e$ is the internal energy of the material, $v$ is the relative volume ($V/V_0$), and $A$, $B$, $R_1$, $R_2$, and $w$ are material constants [49]. The JWL EOS constants for all high explosives used in the ALE3D simulations are shown in Table 4.5.

Table 4.5: Material JWL EOS Coefficients [50]

<table>
<thead>
<tr>
<th>Material</th>
<th>A</th>
<th>B</th>
<th>$R_1$</th>
<th>$R_2$</th>
<th>$w$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETN (50% TMD)</td>
<td>3.46</td>
<td>0.11288</td>
<td>7</td>
<td>2</td>
<td>0.24</td>
</tr>
<tr>
<td>PBX-9407 (90% TMD)</td>
<td>5.73187</td>
<td>0.14639</td>
<td>4.6</td>
<td>1.4</td>
<td>0.32</td>
</tr>
<tr>
<td>Detasheet-C</td>
<td>3.49</td>
<td>0.04524</td>
<td>4.1</td>
<td>1.2</td>
<td>0.3</td>
</tr>
</tbody>
</table>

4.2.7 Burn Parameters

The high explosives were controlled using several burn parameters. The detonator explosives (PETN and RBX-9407) were simultaneously initiated at their centers along the centerline $y=0$ at $t=0$. The resulting detonation shock wave initiates the Detasheet-C explosive. The detonation and burn properties of the high explosives are shown in Table 4.6. The Chapman-Jouguet (CJ) condition is a steady state detonation condition where the flow is sonic. The CJ condition can be determined by locating the point where the Raleigh line and P-v Hugoniot are tangent and their slopes are equal [53]. Any condition less than the CJ point will not produce a detonation shock wave. The following CJ properties for the high explosives were
determined using a code called Cheetah. Element Length is the characteristic size of the elements contained in the HE. Beta is defined as one plus the adiabatic index at the CJ state. Burn Duration is the time interval over which an element burns. Burn Velocity is defined as the CJ detonation velocity. Delay is the time delay set to initiate the explosives, and Lighting Type is the method for defining how an explosive is burned based on its geometry and other features. Lund lighting allows the explosive to propagate outwards from the detonation point (in this case, detonation initiates from the detonator explosives).

Table 4.6: HE detonation properties and burn constants

<table>
<thead>
<tr>
<th>Properties</th>
<th>PETN</th>
<th>PBX-9407</th>
<th>Detasheet-C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [g/cm³]</td>
<td>0.88</td>
<td>1.6</td>
<td>1.48</td>
</tr>
<tr>
<td>$D_{CJ}$ [cm/µs]</td>
<td>0.507</td>
<td>0.794</td>
<td>0.719</td>
</tr>
<tr>
<td>$P_{CJ}$ [Mbar]</td>
<td>0.061</td>
<td>0.268</td>
<td>0.207</td>
</tr>
<tr>
<td>Element Length [cm]</td>
<td>0.027</td>
<td>0.027</td>
<td>0.027</td>
</tr>
<tr>
<td>Beta</td>
<td>3.668</td>
<td>3.766</td>
<td>3.691</td>
</tr>
<tr>
<td>Burn Duration [µs]</td>
<td>0.0526</td>
<td>0.0336</td>
<td>0.0371</td>
</tr>
<tr>
<td>Burn Velocity [cm/µs]</td>
<td>$D_{CJ}$</td>
<td>$D_{CJ}$</td>
<td>$D_{CJ}$</td>
</tr>
<tr>
<td>Delay [µs]</td>
<td>0.0</td>
<td>0.0</td>
<td>n/a</td>
</tr>
<tr>
<td>Lighting Type</td>
<td>Lund</td>
<td>Lund</td>
<td>Lund</td>
</tr>
</tbody>
</table>

4.3 Simulation Results

The tabulated simulation results for water and JP-10 can be seen in Tables 4.7 and 4.8. The nozzle numbers are listed in a similar manner to the experiment for comparison purposes later in this thesis. As expected, the jet velocity and shock velocity for JP-10 increased as the amount of HE increased. As the mass of HE doubled, the shock velocity increased by about 7%, and the jet velocity increased by about 34% for JP-10. One can notice that the shock velocity is less than the jet velocity for Nozzle 5. This has the same behavior as seen in the experiment.

The velocity profile for all nozzles at 50 µs can be seen in Figs. 4.4 and 4.5. The figures are aligned vertically and are axisymmetric in order to fit the page. Each image in the figures has its own legend located on the lower left hand side. As expected, the velocity peaks at


Table 4.7: Simulation Results for Water

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.50</td>
<td>10.90</td>
<td>0.2510</td>
<td>0.1524</td>
</tr>
</tbody>
</table>

Table 4.8: Simulation Results for JP-10

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2 &amp; 3</td>
<td>1.50</td>
<td>10.01</td>
<td>0.2413</td>
<td>0.1685</td>
</tr>
<tr>
<td>4</td>
<td>3.00</td>
<td>9.20</td>
<td>0.2582</td>
<td>0.2472</td>
</tr>
<tr>
<td>5</td>
<td>4.51</td>
<td>8.25</td>
<td>0.2762</td>
<td>0.3310</td>
</tr>
</tbody>
</table>

the jet tip and decreases down into the throat of the nozzle. The geometry of the jets show a thin “stretched” portion where the velocity gradient is high. At locations nearer to the nozzle outlet, the jet bulges outwards and is mainly due to pressure gradients originating from the nozzle interior. Since the pressure gradients increase as more HE is used, the base of the jets in Nozzles 4 and 5 get much thicker and appear to be more turbulent than Nozzles 1 and 2&3. There is also an air shock that formed ahead of the jet tips. One can get a better representation of this by viewing profiles of mach number, velocity, and pressure that can be seen in Appendix C, where the sonic velocity is shown as a black line. The jet tips are round due to the shearing effect of the surrounding air shock. Also,

The deformation of the nozzle, mitigator, and baseplate are clearly visible. The most deformation occurred at the top of the nozzle near the outlet. The stainless steel yield stress was exceeded near the nozzle outlet causing the outlet diameter to increase. Therefore, the jet diameter near the nozzle outlet is slightly thicker than the original outlet diameter at \( t = 0\mu s \). The steel baseplate deformed slightly from the HE detonation products. The deformation was greatest, however, in Nozzles 4 and 5, where the most HE was used. In all four simulations, the lucite mitigator deformed in a similar manner. The mitigator bent from the centerline to the inner nozzle wall, and some small pieces of the mitigator can be seen on the nozzle wall as it scraped against it.
Figure 4.4: Velocity profiles of Nozzle Numbers 1 (left) and 2 (right) at 50 µs
Figure 4.5: Velocity profiles of Nozzle Numbers 4 (left) and 5 (right) at 50 µs
A comparison between Nozzle 1 containing water and Nozzle 2 containing JP-10 with the same amount of HE is shown in Fig. 4.6. The deformation of the solid materials are almost identical for both nozzles. The geometry of the jets are slightly different, however. Since the velocity of the JP-10 jet is larger, the jet extends further away from the nozzle outlet. The wider, bulged section of the water jet contains features that are dissimilar to the JP-10 jet. Also, the tip of the water jet is rounded with a sharp edge along the surface. The JP-10 jet tip is also round, but does not have a defined edge at the base of the tip.

Figure 4.6: Material boundaries of Nozzle Numbers 1 (top) and 2 (bottom) at 50 µs
4.4 Simulation Parameter Study

4.4.1 Setup and Geometry Variations

A parameter study was conducted on the baseline simulations to determine the most effective geometry to produce the highest jet velocity. The parameter study was conducted using the liquid, JP-10, at constant volume. All geometrical dimensions were kept constant except the nozzle angle, nozzle outlet diameter, and the total height of the nozzle. Since the volume of JP-10 was held constant and the nozzle angle and outlet diameter were changed, the total height was forced to change as well. The mass of HE was also constant for all simulations at 1.46 grams (not including the explosives contained in the detonator). A total of six simulations were performed for this study. The nozzle angle was changed between 30°, 45°, and 60° from the centerline. For each nozzle angle, the nozzle outlet diameter was changed from 0.1875 inch (3/16 inch) to 0.25 inch.

4.4.2 Parameter Variation Results

The results for this parameter study are shown in Table 4.9. The jet tip velocity was recorded at approximately one inch or 2.54 cm from the leading edge of the nozzle along the centerline (x-axis). Also, the maximum internal nozzle pressure within the JP-10 was provided to see if there is any correlation.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>BASELINE1</td>
<td>30°</td>
<td>0.1875</td>
<td>0.1694</td>
<td>0.0491</td>
</tr>
<tr>
<td>BASELINE2</td>
<td>30°</td>
<td>0.25</td>
<td>0.1543</td>
<td>0.0466</td>
</tr>
<tr>
<td>BASELINE3</td>
<td>45°</td>
<td>0.1875</td>
<td>0.1693</td>
<td>0.1163</td>
</tr>
<tr>
<td>BASELINE4</td>
<td>45°</td>
<td>0.25</td>
<td>0.1640</td>
<td>0.1048</td>
</tr>
<tr>
<td>BASELINE5</td>
<td>60°</td>
<td>0.1875</td>
<td>0.1467</td>
<td>0.1162</td>
</tr>
<tr>
<td>BASELINE6</td>
<td>60°</td>
<td>0.25</td>
<td>0.1413</td>
<td>0.1059</td>
</tr>
</tbody>
</table>

The highest jet tip velocities were observed in BASELINE1 and BASELINE3 to be 0.1694 cm/µs and 0.1693 cm/µs, respectively. Both nozzle geometries had an outlet diameter of
3/16 inch, and a nozzle angle of 30° and 45°, respectively. An interesting thing to note is that the maximum internal pressure for the 45° nozzles were over twice that of the 30° nozzles. This doesn’t seem logical because the jet velocities are almost identical. The reason for this lies within the nozzle where the initial shock wave traveling through the JP-10 reflects off the nozzle inner wall, and creates a large or small jump in pressure. The lowest jet velocities were observed in the 60° nozzles. Again, the internal pressure doesn’t correlate with the rest of the results. Thus, it appears that there is no correlation with maximum internal pressure and jet tip velocity. All in all, the parameter study has proven that the geometry of the original baseline simulations was the most effective in producing large jet tip velocities.
Chapter 5

Experiment and Simulation Comparison

5.1 Comparison Results

The ALE3D simulations were compared to the experiment results. Tables 5.1 and 5.2 list the percent change between the experiment and simulation results for water and JP-10. The change in initial mass of HE and initial mass of water and JP-10 is minimal. The change in shock velocity for water is very low, and is expected because the EOS parameters were taken from literature. This result is much better than the shock velocity for JP-10. The simulation shock velocity for all JP-10 simulations were between 11.5%-19.6% less than in the experiment. This means that the Grüneisen parameters fit from the Helmholtz EOS of JP-10 need improvement. Also, the jet velocity in all simulations were between 46%-54% lower than in the experiment. This large difference can be the result of several hypotheses. First, the resolution of the simulations were not as low as desired, meaning that the viscosity and surface forces could have limited the jet from achieving more realistic results. Also, the EOS for JP-10 and water might not be accurate at low pressures and densities once the jet expands into atmosphere.

Nonetheless, the simulation jet velocity should have been greater than in the experiment because the simulation assumes perfect conditions. The geometry in the simulations contain no defects and are perfectly symmetrical. Also, the nozzles in the simulation were perfectly sealed against the baseplate, whereas in the experiment, the nozzles were held to the baseplate via screws. Thus, part of the HE product gases were allowed to escape the underside of the nozzle in the experiment. Again, the simulation didn’t allow this to happen, so all of
Table 5.1: Percent change between experiment and simulation results for Water

<table>
<thead>
<tr>
<th>Nozzle Number</th>
<th>Change in Mass of HE</th>
<th>Change in Mass of Water</th>
<th>Change in Shock Velocity</th>
<th>Change in Jet Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.67%</td>
<td>3.0%</td>
<td>1.21%</td>
<td>-46.9%</td>
</tr>
</tbody>
</table>

Table 5.2: Percent change between experiment and simulation results for JP-10

<table>
<thead>
<tr>
<th>Nozzle Number</th>
<th>Change in Mass of HE</th>
<th>Change in Mass of JP-10</th>
<th>Change in Shock Velocity</th>
<th>Change in Jet Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-0.66%</td>
<td>2.67%</td>
<td>-16.2%</td>
<td>-51.0%</td>
</tr>
<tr>
<td>3</td>
<td>0%</td>
<td>1.11%</td>
<td>n/a</td>
<td>-53.8%</td>
</tr>
<tr>
<td>4</td>
<td>0.33%</td>
<td>2.68%</td>
<td>-19.6%</td>
<td>-46.0%</td>
</tr>
<tr>
<td>5</td>
<td>2.27%</td>
<td>4.43%</td>
<td>-11.5%</td>
<td>n/a</td>
</tr>
</tbody>
</table>

The HE product gases expanded into the liquid, and out the detonator hole.

The outline of the nozzles and jets from the experiment and simulations are shown in Figs. 5.1-5.3. A single frame from Nozzles 1, 2, and 4 in the experiment is compared to the same time in the simulations. Nozzle 3 contained the same amount of HE as Nozzle 2, and the shape of the jet was lacking symmetry, hinting that there might have been an abnormality in the geometry of the nozzle. Thus, Nozzle 3 was not compared in these figures. The experiment high-speed images of Nozzle 5 were inconclusive and were not compared to the simulation, neither. Although, the second frame from Nozzle 5 could have been compared, but the time delay was too short and the JP-10 did not exit the nozzle in the simulation. One can see that the jets from the simulations are much shorter and thinner than in the experiment. However, the jets from simulation still have the basic shape of the jets from the experiment. They all contain a thinner ”stretched” region on top of a thicker bulged region. If the jet velocities from the simulation were analogous to the experiment, the geometry of the jets would appear much more similar to one another. Although the results are not an exact comparison, they are still important for this study and should not be considered trivial.

The geometry of the stainless steel nozzles are almost identical to one another. Along
the top surface of the nozzle near the outlet, the nozzle bends upwards. These bent regions of the nozzles are a close match to the experiment results. This means that the nozzle material properties and EOS parameters were defined appropriately. Yet, the nozzles in the experiment fractured into four or more pieces (not shown in this section), but the simulation nozzles did not fracture at all. A more accurate fracture model would solve this issue for the stainless steel model.

Figure 5.1: Nozzle and jet outline from experiment (left) and simulation (right) for Nozzle 1 with $\sim 1.50$ g HE and $\sim 10.9$ g water
Figure 5.2: Nozzle and jet outline from experiment (left) and simulation (right) for Nozzle 2 with $\sim 1.51$ g HE and $\sim 10$ g JP-10

Figure 5.3: Nozzle and jet outline from experiment (left) and simulation (right) for Nozzle 4 with $\sim 3$ g HE and $\sim 9.2$ g JP-10
Chapter 6

Expansion Fan Analysis of JP-10 Jet

The JP-10 jet from the ALE3D simulations can be modeled numerically using a one dimensional expansion fan (rarefaction) self-similar analysis. Knowing the initial fluid properties such as velocity, pressure, and density at the nozzle exit, one can determine the final state properties as a function of time and position using the following flow analysis technique.

6.1 Riemann Invariant

An adiabatic expansion or rarefaction occurs when a fluid at high pressure and density suddenly expands to a low pressure, density state. This often occurs from a shock wave passing through a fluid produced by high explosives, a shock tube, or other means. The best method for modeling rarefactions is by deriving characteristics and the Riemann invariants. Derived from the equations of motion, characteristics are fluid particle paths of sound waves that appear on an x-t diagram [6, 34, 35]. Riemann invariants are quantities that remain constant along the path of the characteristics, assuming constant-area flow with negligible body forces (gravitational forces aren’t considered due to the large pressure change). In our case, we will list the characteristics and Riemann invariants assuming one-dimensional isentropic flow.

The characteristics of the fluid path for disturbances propagating at the sound speed is defined by

\[ C_{\pm} : \frac{dx}{dt} = u \pm a, \]  

(6.1)

where \( a = \sqrt{\left(\frac{\partial u}{\partial p}\right)_s} \), and for disturbances propagating at the fluid velocity described by

\[ C_0 : \frac{\partial x}{\partial t} = u. \]  

(6.2)
It is required that the equations of motion are to be put into the desired form that is relevant to the propagation along the characteristics. First, one can recall that the derivative of a function \( f(x, t) \) defining an arbitrary curve \( x = \omega(t) \) is

\[
\left( \frac{\partial f}{\partial t} \right)_{\omega} = \frac{df}{dt} + \frac{dx}{dt} \frac{\partial f}{\partial x}.
\] (6.3)

The remaining derivation is easier to complete if one solves in terms of pressure instead of density. One can convert density into pressure by using the following equation derived from the definition of sound speed.

\[
d\rho = \left( \frac{\partial \rho}{\partial P} \right)_{S=\text{constant}} dP = \frac{dP}{a^2} \] (6.4)

One can substitute the latter into the continuity and momentum equations (Eqs. 2.11 and 2.12) to obtain:

\[
\frac{1}{\rho a} \frac{\partial P}{\partial t} + \frac{u}{\rho a} \frac{\partial P}{\partial x} + a \frac{\partial u}{\partial x} = 0 \] (6.5)

and

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial P}{\partial x} = 0. \] (6.6)

Adding Euler’s equation (conservation of momentum) to the above momentum equation, one can develop an equation into the desired form similar to Eq. 6.3.

\[
\left[ \frac{\partial u}{\partial t} + (u \pm a) \frac{\partial u}{\partial x} \right] \pm \frac{1}{\rho a} \left[ \frac{\partial P}{\partial t} + (u \pm a) \frac{\partial P}{\partial x} \right] = 0 \] (6.7)

The full set of characteristic equations for planar, one-dimensional and isentropic flow, can be written as [6, 34, 35]

\[
dJ_{\pm} \equiv du \pm \frac{dp}{\rho a} = 0 \quad \text{on} \quad C_{\pm} : \frac{dx}{dt} = u \pm a, \] (6.8)

\[
\frac{\partial S}{\partial t} = 0 \quad \text{on} \quad C_0 : \frac{\partial x}{\partial t} = u. \] (6.9)

Integrating Eq. 6.8 produces the Riemann invariants \( J_{\pm} \) shown as:

\[
J_{\pm} = u \pm \int \frac{dp}{\rho a} \] (6.10)

or in terms of density [34]:

\[
J_{\pm} = \int \frac{a(\rho)d\rho}{\rho} \pm u \] (6.11)

The Riemann invariants are indefinite integrals that remain constant along each characteristic for simple wave flow. For example, the Riemann invariant, \( J_+ \), is constant along
the characteristic, $C_+$, and the same applies for $J_-$ and $C_-$. If one Riemann invariant is constant over some region, then the characteristics for the other Riemann invariant as they cross this region are straight lines [6]. Density, $\rho$, and sound speed, $a$, are required in Eq. 6.10 because they are functions of pressure. Only velocity, $u$, and one other quantity are required to specify any other state of the fluid. Thus, $J_+$ and $J_-$ can fully specify the state of a fluid, which greatly simplifies the flow analysis. To add, the flow properties such as pressure, density, and velocity remain constant along each characteristic, and the properties of a fluid at the intersection of $J_\pm$ and $C_\pm$ can also be determined. For simple waves where $u$ and $a$ are constant, the characteristics are linear.

### 6.2 Ideal Flow Analysis

One can perform this flow analysis using an ideal EOS to better understand the simple wave theory. The classical form of the EOS for a perfect gas is

$$e = \frac{p}{\rho(\gamma - 1)},$$

(6.12)

where $\gamma$ is the adiabatic index (specific heat ratio) expressed as $\gamma = c_p/c_v$. The specific heat capacity per unit mass at constant pressure and volume are written as $c_p$ and $c_v$, respectively. Temperature can be solved by substituting the internal energy per unit mass, $e = c_v T$, into the ideal EOS to obtain

$$T = \frac{p}{\rho(\gamma - 1)c_v}.$$  

(6.13)

#### 6.2.1 Entropy

The thermodynamic entropy $S(e, v)$ is defined by the equation [10]

$$dS = \frac{de}{T} + \frac{p}{T}dv.$$  

(6.14)

Eq. 6.12 can be differentiated and solved for $de$ and $dv$ to obtain

$$de = \frac{1}{\rho(\gamma - 1)}dp - \frac{p}{\rho^2(\gamma - 1)}d\rho \quad \text{and} \quad dv = -\frac{1}{\rho^2}d\rho.$$  

(6.15)

The latter can be substituted into the entropy equation along with Eq. 6.13 to obtain

$$ds = \frac{\rho(\gamma - 1)c_v}{p} \left[ \frac{1}{\rho(\gamma - 1)}dp - \frac{p}{\rho^2(\gamma - 1)}d\rho \right] - \frac{\rho(\gamma - 1)c_v}{\rho^2}d\rho,$$

(6.16)
which reduces to
\[
ds = c_v \left( \frac{dp}{p} - \frac{\gamma d\rho}{\rho} \right). \tag{6.17}
\]
Now that the differential is decoupled, one integrates the latter to obtain a function for entropy of an ideal gas,
\[
S(\rho, p) = S_0 + c_v \log(p\rho^{-\gamma}). \tag{6.18}
\]

### 6.2.2 Isentropes and Riemann Invariants

One can define \( \kappa = \exp[(S(\rho, p) - S_0)/c_v] \) and solve for \( p \) to get the isentrope for an ideal, polytropic gas,
\[
p = \kappa \rho^\gamma. \tag{6.19}
\]
An isentrope is a curve relating two variables along which the entropy is constant [10]. However, one can find a simple relationship for isentropic flow of a polytropic gas as
\[
p = p_0 \left( \frac{\rho}{\rho_0} \right)^\gamma. \tag{6.20}
\]
With this in mind, one can derive the sound speed of an ideal, polytropic gas using the definition of sound speed, \( a = \sqrt{\frac{\partial p}{\partial \rho}} \), and is shown as [34, 54]
\[
a = \sqrt{\kappa \gamma \rho^\gamma - 1} = \sqrt{\frac{\gamma p_0}{p}} = \sqrt{\gamma \frac{p_0}{p_0} \left( \frac{\rho_0}{\rho} \right) \frac{\gamma - 1}{2}}, \tag{6.21}
\]
where \( a_0 \) is the initial sound speed of the fluid defined as \( a_0 = \sqrt{\gamma p_0/\rho_0} \). The sound speed is substituted into Eq. 6.10, and integrated to obtain the Riemann invariants
\[
J_+ = u + \frac{2}{\gamma - 1} a \quad \text{and} \quad J_- = u - \frac{2}{\gamma - 1} a, \tag{6.22}
\]
which are constant along the characteristics
\[
C_\pm : \frac{dx}{dt} = u \pm a. \tag{6.23}
\]

### 6.2.3 Rarefaction Fan

An adiabatic rarefaction is produced when a fluid experiences a large decrease in pressure and density, often to standard atmospheric conditions. Unlike a shock wave where the
compression wave moves in the same direction as the dynamic fluid, a rarefaction wave moves in the opposite direction of the moving fluid. Also, the sound speed, pressure, and density decrease in a rarefaction wave, opposite of a compression wave. In the following example, the high pressure-density state will be created by a shock wave traveling through a polytropic gas.

The image below shows the characteristics of a planar adiabatic rarefaction wave centered at the origin. In this example, one assumes that a uniform fluid initially at rest (left of the origin), is bordered by a piston that instantaneously accelerates to velocity, $U$, and travels the opposite direction of the fluid ($+x$ direction). However, for this project, one can assume that there is no longer a piston, but instead, there is a surrounding fluid at vacuum. A strong shock wave then passes through the fluid at shock velocity $u_s$, and fluid particle velocity, $u_p$. The fluid particle velocity now acts as the ”piston” velocity, $U = u_p$. The characteristics to the left of the trailing edge represent the initial medium (low dense, high velocity gas outside of the nozzle). The trailing edge is the tail of the rarefaction wave that propagates at the sound speed of the initial medium. The leading edge is the front of the region of expansion and the characteristics are constant. Lastly, the $C_-$ characteristics between the leading and trailing edges form a fan which emerge from the origin and is considered the rarefaction or expansion fan [6, 34, 35].

![Figure 6.1: Planar, adiabatic rarefaction fan characteristics [6]](image)

It is desired to determine the properties of the fluid flow from the $C_-$ characteristics because they are linear, unlike the $C_+$ characteristics within the rarefaction fan. The $C_-$
characteristics are shown

\[
\text{for } x \leq \text{Trailing edge, } C_- : \frac{dx}{dt} = -a,
\]

\[
\text{for } x \geq \text{Leading edge, } C_- : \frac{dx}{dt} = U - a,
\]

within the Rarefaction fan, \( C_- : \frac{dx}{dt} = u - a. \)  \( (6.24) \)

However, since the Riemann invariant \( J_+ \) is constant everywhere along \( C_+ \) when \( t = 0 \), \( C_- \) is also constant. When \( u = 0 \), the sound speed \( a = a_0 \), which leads to

\[
J_+ = u + \frac{2}{\gamma - 1} a = \frac{2a_0}{\gamma - 1}.
\]

Solving for \( a \), one can obtain an equation for sound speed for a polytropic gas as a function of initial sound speed, \( a_0 \), specific heat ratio, \( \gamma \), and fluid velocity, \( u \), as \([6, 34]\)

\[
a = a_0 - \frac{\gamma - 1}{2} u. \quad (6.26)
\]

The \( C_- \) characteristics can now be functions of the initial sound speed, \( a_0 \), instead of instantaneous sound speed, \( a \), when the latter is substituted into Eq: 6.24,

\[
\text{for } x \leq \text{Trailing edge: } \frac{dx}{dt} = \frac{\gamma - 1}{2} u - a_0,
\]

\[
\text{for } x \geq \text{Leading edge: } \frac{dx}{dt} = \frac{\gamma + 1}{2} U - a_0,
\]

within the Rarefaction fan: \( \frac{dx}{dt} = \frac{\gamma + 1}{2} u - a_0. \)  \( (6.27) \)

The \( C_- \) characteristic within the rarefaction fan can be integrated to find the fluid velocity across an expansion fan as a function of \( x/t \):

\[
u = \frac{2}{\gamma + 1} \left( a_0 + \frac{x}{t} \right). \quad (6.28)
\]

One can continue to determine the other properties for a polytropic gas through the expansion fan using the following isentropic relations for an ideal, polytropic gas \([6]\):

\[
\frac{\rho}{\rho_0} = \left( \frac{a}{a_0} \right)^{2/(\gamma - 1)} \quad \text{and} \quad \frac{p}{p_0} = \left( \frac{a}{a_0} \right)^{2\gamma/(\gamma - 1)},
\]

\( (6.29) \)

and

\[
\frac{\rho}{\rho_0} = \left( 1 - \frac{(\gamma - 1)u}{2a_0} \right)^{2/(\gamma - 1)} \quad \text{and} \quad \frac{p}{p_0} = \left( 1 - \frac{(\gamma - 1)u}{2a_0} \right)^{2\gamma/(\gamma - 1)}.
\]

\( (6.30) \)
Lastly, Eq. 6.28 can be substituted into the latter to obtain the desired relationships for density and pressure across an expansion fan of a polytropic gas:

$$\frac{\rho}{\rho_0} = \left(\frac{2}{\gamma + 1} - \frac{\gamma - 1}{\gamma + 1} \frac{x}{a_0 t}\right)^{2/(\gamma - 1)}$$  \hspace{1cm} (6.31)

$$\frac{p}{p_0} = \left(\frac{2}{\gamma + 1} - \frac{\gamma - 1}{\gamma + 1} \frac{x}{a_0 t}\right)^{2\gamma/(\gamma - 1)}$$  \hspace{1cm} (6.32)

for

$$-a_0 t \leq x \leq \frac{\gamma + 1}{2} U t - a_0 t \leq \frac{2}{\gamma - 1} a_0 t.$$  \hspace{1cm} (6.33)

### 6.3 Numerical Method for Non-ideal EOS

The analytical solution to the flow analysis in section 6.2 is only achievable for simple EOS’s such as the ideal EOS. However, the ideal EOS is not valid for many fluids and more complex EOS’s are needed. Non-ideal EOS’s used to define fluid properties typically contain several terms. For example, the Gruneisen EOS shown in Eq. 4.1 has several terms that prohibit the equation to be analytically solved in this manner. Thus, an analytical solution to the rarefaction analysis is not possible for many non-ideal EOS’s. Numerical methods are required to solve the expansion fan problem for a non-ideal EOS.

#### 6.3.1 Self Similar 1D Euler Solution

The simple, one dimensional Euler equations, derived from Eq. 2.11 - 2.12 assuming that viscosity and body forces due to gravity are neglected, are shown as:

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0,$$  \hspace{1cm} (6.34)

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0,$$  \hspace{1cm} (6.35)

$$\frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + \rho a^2 \frac{\partial u}{\partial x} = 0,$$  \hspace{1cm} (6.36)

where the sound speed $a$ can be manipulated as a function of energy [55],

$$a = \left(\frac{p - \rho^2 \frac{\partial e}{\partial \rho}}{\rho^2 \frac{\partial e}{\partial p}}\right)^{1/2}.$$  \hspace{1cm} (6.37)
Assuming that $\rho, u$, and $p$ are self-similar, one can define $\xi = x/t$, then, $\rho, u$, and $p$ are only functions of $\xi$. Since $a$ is dependent on $\rho$ and $p$, one can also assume that $a$ is dependent solely on $\xi$ [56]. Via the chain rule, one can note that

$$
\frac{\partial \rho(x,t)}{\partial x} = \frac{1}{t} \frac{d \rho(\xi)}{d \xi} \quad \text{and} \quad \frac{\partial \rho(x,t)}{\partial t} = -\frac{x}{t^2} \frac{d \rho(\xi)}{d \xi}.
$$

(6.38)

With this in mind, the Euler equations simplify to

$$
(u - \xi)\rho' + \rho u' = 0,
$$

(6.39)

$$
(u - \xi)\rho u' + p' = 0,
$$

(6.40)

$$
(u - \xi)p' + a^2 \rho u' = 0.
$$

(6.41)

One can express these equations in matrix form as

$$
\begin{pmatrix}
\rho' \\
u' \\
p'
\end{pmatrix} =
\begin{pmatrix}
(u - \xi) & \rho & 0 \\
0 & (u - \xi)\rho & 1 \\
0 & a^2 \rho & u - \xi
\end{pmatrix}
\begin{pmatrix}
\rho \\
u \\
p
\end{pmatrix}.
$$

(6.42)

This is a set of homogeneous ordinary differential equations (ODE’s), and any numerical method requires solving these equations for $\rho', u', p'$. In order for a nontrivial solution to exist, the matrix must be singular, meaning that the determinate must equal zero. The determinant of this matrix is

$$
(u - \xi)(u - \xi - a)(u + \xi - a)\rho = 0.
$$

(6.43)

The latter equation is satisfied if $u = \xi$, $u = a \pm \xi$, or $\rho = 0$. However, the only solution that makes physical sense is if $u = a + \xi$, or

$$
u = a + \frac{x}{t}.
$$

(6.44)

This is a conclusion that has already been obtained from the Riemann analysis in the previous section. Substituting this back into the self-similar Euler equations, one finds

$$
a\rho' + \rho(1 + a') = 0,
$$

(6.45)

$$
a\rho(1 + a') + p' = 0,
$$

(6.46)

$$
a^2 \rho(1 + a') + ap' = 0.
$$

(6.47)

Note that the second and third equations are redundant, so one takes the first two equations and solves for $\rho'$ and $p'$ shown as

$$
\rho'(\xi) = -\rho(\xi) \frac{1 + a'(\xi)}{a(\xi)},
$$

(6.48)

$$
p'(\xi) = -\rho(\xi)a(\xi)(1 + a'(\xi)).
$$

(6.49)
6.3.2 Steps for Solving the Model

A numerical method for solving this problem proceeds as follows. First, one determines the sound speed equations $a(\xi)$ and $a'(\xi)$ based on $\rho(\xi)$ and $p(\xi)$ using any EOS. Next, $a(\xi)$ and $a'(\xi)$ are substituted into Eq’s. 6.48 - 6.49 and solved for $\rho'$ and $p'$ using a numerical solving technique in any mathematics computing software such as Wolfram Mathematica. The simplest boundary conditions to use are the trailing edge characteristics, at $x = -a_0 t$ or $\xi = -a_0$, at which $\rho = \rho_0$ and $p = p_0$. The ODEs should be integrated up to $\xi = U + a_0$, where $U$ is the post-shocked fluid particle velocity. Once density, $\rho$, and pressure, $p$, are solved, one can compute the sound speed of the fluid, $a$, and fluid velocity, $u$.

6.4 ALE3D and Expansion Fan Results Comparison

The numerical method described in the previous section was used to solve the flow analysis of a rarefaction fan for JP-10, and is compared to the ALE3D simulation results. The rarefaction fan was solved using the Grüneisen EOS from Eq. 4.1 and the material parameters for JP-10 from Table 4.3. The initial conditions to solve this problem were determined from the simulation results from Nozzle Number 2. The initial pressure, density, and fluid velocity were determined at the nozzle exit along the centerline. A time average was performed on these properties to reduce any large sudden changes. The initial pressure, density, and velocity are 0.015 Mbar, $1.1 \text{ g/cm}^3$, and $0.06 \text{ cm/\mu s}$, respectively. Sound speed was calculated from Eq. 6.37 and is 0.2407 $\text{ cm/\mu s}$.

The results for the fluid particle velocity, pressure, and density from the simulation and the rarefaction self similar analysis can be seen in Figs. 6.2-6.4. The rarefaction solution is shown as a black line. Simulation time history results were recorded at nodes along the centerline from the leading edge of the lucite mitigator, to the leading edge of the JP-10 jet tip. Some post processing was performed on the ALE3D simulation results to achieve the desired form for comparison purposes. First, the raw data was time averaged to reduce any large spikes in data. Since $\rho$, $u$, and $p$ were assumed to be self-similar, the simulation results had to be transformed into a self-similar form as well. One can see that the x-axis label is $\xi = (x - x_0)/(t - t_0)$. The values for $x_0$ and $t_0$ were determined by trial and error until the simulation data overlapped one another. These values came out to be 4.99 cm and 0.0 $\mu s$, respectively. The location of the nozzle exit is at $\xi=0$, and the rarefaction fan is centered at $\xi=0.5$.

One can see that the comparisons are similar, but not exact. The slope of the rarefaction
velocity is much lower than the simulation result, and extends well into what would be the nozzle interior. In reality, the greatest acceleration in velocity would be located near the nozzle exit, shown in the simulation. Also, the expansion fan velocity is greater than the simulation result by about 0.02 cm/µs, which is not trivial. The rarefaction pressure does not decrease as quickly as in the simulation. One should note that the simulation pressure dips below zero megabar into negative pressures. The rarefaction analysis approaches zero pressure, so the sub-zero pressures from the simulation were not comparable. The density results were slightly better. The rarefaction density follows the simulation results much better, yet, the slope of the line is still too low.

Figure 6.2: Expansion Fan Velocity Results
Pressure Expansion Fan Results

\[ \xi = \frac{x-x_0}{t-t_0} \text{ (cm/µs)} \]

Pressure (Mbar)

\[ t = 15 \, \mu s \]
\[ t = 16 \, \mu s \]
\[ t = 17 \, \mu s \]
\[ t = 18 \, \mu s \]

Figure 6.3: Expansion Fan Pressure Results

Density Expansion Fan Results

\[ \xi = \frac{x-x_0}{t-t_0} \text{ (cm/µs)} \]

Density (g/cm\(^3\))

\[ t = 15 \, \mu s \]
\[ t = 16 \, \mu s \]
\[ t = 17 \, \mu s \]
\[ t = 18 \, \mu s \]

Figure 6.4: Expansion Fan Density Results
Chapter 7

Conclusion and Future Studies

At first, the motivation and applications were discussed, as well as some aviation fuel types. Past experiment and simulation results were reported for equation of state studies and supersonic liquid jets. The physical properties, chemical structure, and equation of state of JP-10 was discussed. The shock relations for JP-10 were determined using the Helmholtz EOS of JP-10.

An experiment was performed with Prof. Nick Glumac to achieve rapid decompression of JP-10 and water via a converging nozzle. The shock velocities within the JP-10 or water filled nozzle, and the resulting jet velocities increased as the amount of HE increased. A high-speed framing camera captured images of the JP-10 jet formation for each nozzle, and showed that the jet tip stretched ahead of a wider, bulged region.

A simulation of each nozzle from the experiment was performed in ALE3D using similar materials, geometry, and dimensions. A parameter study was performed on the nozzle angle and outlet diameter to see how the jet velocity and internal pressure was affected. A nozzle angle of 45 degrees and an outlet diameter of 0.1875 inch created the highest jet velocities and internal pressures.

The results of the simulations were compared to the experiment results and showed some disagreement. The JP-10 simulation results for shock velocity were within 20% of the experiment results. The jet velocities in the simulation were about half the experiment jet velocities. Water showed the best comparison with a shock and jet velocity within 1.2% and 47%, respectively. The geometry of the jets in the simulations were thinner and shorter than in the experiment, but, they showed similar features.

Lastly, a numerical expansion fan model was discussed for JP-10 using the Grüneisen EOS from ALE3D. Self-similar numerical results for velocity, pressure, and density were
compared to the ALE3D nozzle results. The numerical model showed some agreement with the ALE3D simulation results, however, the comparison still needs improvement.
Appendix A - Nozzle Dimensions

Figure A.1: Nozzle dimensions shown in inches
Figure A.2: PMMA mitigator dimensions shown in inches
Figure A.3: Baseplate dimensions shown in inches
Appendix B - High-Speed Images of Liquid Jets

Figure B.1: High-speed Images of Nozzle 1, with 1.49 g HE and 10.58 g water
Figure B.2: High-speed Images of Nozzle 2, with 1.51 g HE and 9.75 g JP-10

Figure B.3: High-speed Images of Nozzle 3, with 1.50 g HE and 9.90 g JP-10
Figure B.4: High-speed Images of Nozzle 4, with 2.99 g HE and 8.96 g JP-10

Figure B.5: High-speed Images of Nozzle 5, with 4.41 g HE and 7.90 g JP-10
Appendix C - Mach, Velocity, and Pressure Results

Figure C.1: Mach profiles of Nozzle Numbers 1 (left) and 2 (right) at 50 µs

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Figure C.2: Mach profiles of Nozzle Numbers 4 (left) and 5 (right) at 50 µs
Figure C.3: Velocity contour profiles of Nozzle Numbers 1 (left) and 2 (right) at 50 \( \mu s \)
Figure C.4: Velocity contour profiles of Nozzle Numbers 4 (left) and 5 (right) at 50 $\mu$s
Figure C.5: Pressure contour profiles of Nozzle Numbers 1 (left) and 2 (right) at 50 $\mu$s
Figure C.6: Pressure contour profiles of Nozzle Numbers 4 (left) and 5 (right) at 50 µs
Bibliography


