MODELING THE INFLUENCE OF SHOCK WAVES ON THE
COMBUSTION OF ALUMINUM DROPLETS

A Dissertation in
Mechanical Engineering
by
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ABSTRACT

A model for calculating the interaction between shock waves and a reacting aluminum droplet was developed. The model accounts for acoustic impedance mismatch at the liquid surface, droplet deformation, wave propagation in the liquid, and cavitation. To solve this problem, a low-dissipation method for computing reacting gas dynamic flows was developed. This method combines features from the double-flux multi-component model, nonlinear error-controlled WENO, adaptive TVD slope limiters, rotated Riemann solvers, and adaptive mesh refinement to obtain a method that is both robust and accurate. Success of the technique is demonstrated using an extensive series of numerical experiments including premixed deflagrations, Chapman-Jouget detonations, re-shocked Richtmyer-Meshkov instability, shock-wave and hydrogen gas column interaction, and multi-dimensional detonations. An extended Riemann problem accounting for phase change and surface tension was developed to couple a reacting gas to a vaporizing compressible liquid. The numerical method compares well with empirically measured separation locations over spheres, heat transfer correlations, and droplet deformation criterion. The numerical algorithms developed in this work are fairly robust and applicable to a wide variety of compressible chemically reacting flows with or without interface capturing and phase change. Computed results for shock waves interacting with liquid droplets indicate that shock waves reduce evaporation rate for non-reacting Al droplets, while increasing the burning rate when chemical reactions are considered; suggesting that the combustion of aluminum droplets may be kinetically-controlled mechanisms. To the author’s knowledge, this work represents the first time that a compressible reacting gas-dynamic flow has been coupled to a compressible liquid with vaporization and surface tension.
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NOMENCLATURE

Abbreviations

AMR  Adaptive Mesh Refinement
AUSM  Advection Upstream Splitting Method
BC  Boundary Condition
BDF  Backwards Differentiation Formula
CFL  Courant-Friedrichs-Levy
CS  Control Surface
CV  Control Volume
CJ  Chapman-Jouget
EOS  Equation of State
FVS  Flux Vector Splitting
FT  Front Tracking
GFM  Ghost Fluid Method
GOx  Gaseous Oxygen
HEX  High Explosive
HLLC  Harten, Lax, van Leer with Contact
HOUC  High-Order Upstream Central
ILES  Implicit Large Eddy Simulation
LES  Large Eddy Simultion
LLF  Local Lax-Friedrichs
LM   Low Mach
LODI Local One-Dimensional Inviscid
LOx  Liquid Oxygen
LSM  Level Set Method
LWENO Linear Weighted Essentially Non-Oscillatory
m-Isen Modified Isentropic cavitation model
m-Schmidt Modified Schmidt cavitation model
M4   Four parameter minmod
M4X  Six parameter minmod
MD   Median
MM   Minmod
MLP  Multidimensional Limiting Process
Mom  Momentum
MP   Monotonicity Preserving
MPWENO Monotonicity Preserving Weighted Essentially Non-Oscillatory
MUSCL Monotone Upstream-centered Schemes for Conservation Laws
ODE  Ordinary Differential Equation
PDE  Partial Differential Equation
RKC  Runge-Kutta-Chebyshev
RK2  Second Order Runge-Kutta
RK3  Third Order strong stability preserving Runge-Kutta
RM   Richtmyer-Meshkov
RTI  Rayleigh-Taylor Instability
SAMR Structured Adaptive Mesh Refinement
SB  Suberbee
SymBO Symmetric Bandwidth Optimized
TBX Thermobaric Explosive
TKE Turbulent Kinetic Energy
TV  Total Variation
TVD Total Variation Diminishing
VOF Volume of Fluid
WENO Weighted Essentially Non-Oscillatory

**Roman Symbols**

- $a$  Runge-Kutta-Chebyshev parameters, linear interpolation table slope, WENO grid point coefficient, or generic constant
- $A$  Area, pre-exponential factor, or Tait equation of state parameter
- $A_0$ Nucleation parameter
- $At$  Atwood number
- $A$  Flux Jacobian
- $b$  Dummy variable per unit mass, RKC parameters, or linear interpolation constant
- $B$  Spalding transfer number, Tait equation of state parameter, or dummy variable
- $c$  Speed of sound, condensation coefficient, or parameters for calculating interface location
- $c_{det}$ Detonation velocity
- $c_{gs}, c_{ls}$ Modified Schmidt cavitation model parameters
\( \bar{c} \)  Roe averaged sound speed

\( \mathbf{C} \)  Characteristic variable vector

\( C \)  Optimal WENO stencil coefficient, m-Isen model constant, or level set velocity modification function

\( C_d \)  Drag coefficient

\( C_p \)  Constant pressure specific heat

\( C_{m, s, t} \)  Thermophoresis force constants

\( C_v \)  Constant volume specific heat

\( d \)  Diameter, distance function, MP curvature, or parameters for integrating conserved variables at boundaries

\( \mathbf{D} \)  Mass diffusion potential or divided difference

\( D \)  Mass diffusivity

\( Da \)  Damköhler number

\( D_x^0 \)  Level set gradient in x-direction

\( D_{xx}^0 \)  Second derivative of the level set function in x-direction

\( e \)  Total energy (sensible and chemical energies) per unit mass, or error measurement for grid refinement

\( e_i \)  Error for smoothness estimate at cell \( i \)

\( E \)  Total internal energy (sensible, kinetic, and chemical energies) per unit mass

\( E_a \)  Activation energy

\( f \)  Body force

\( \mathbf{f}_{\sigma} \)  Net surface tension force

\( f \)  Number of cells per droplet diameter

\( f_a \)  AUSM parameter

\( f_L \)  Left velocity jump function for the Riemann problem
$F_d$ Drag force factor

$F/O$ Mass fuel to oxidizer ratio

$F$ Inviscid flux in x-direction

$F_d$ Net drag force per unit volume

$F_T$ Thermophoresis force

$F_v$ Viscous flux in x-direction

$F_{\text{vap}}, F_{\text{cond}}$ Cavitation rate constants

$g_R$ Right velocity jump function for the Riemann problem

$G$ Inviscid flux in y-direction

$G_v$ Viscous flux in x-direction

$G_r$ Radial source vector for hyperbolic flux

$h$ Enthalpy

$h_{f,i}^0$ Enthalpy of formation for chemical species $i$

$h_0^m$ Reference enthalpy for the double-flux model

$H$ Stagnation enthalpy, PDE extrapolation speed function, or Heaviside function

$H_E$ PDE extrapolation Hamiltonian

$H_n$ Hamiltonian for the level set method, $H_n = \sqrt{\phi_x^2 + \phi_y^2}$

$\tilde{H}$ Roe averaged stagnation enthalpy

$i$ Species or grid point index

$IS$ WENO candidate stencil smoothness indicator

$J_c$ Nucleation rate

$J_C$ Jump conditions

$J_i$ Molecular collision rate

$J''$ Diffusion species mass flux normal to surface

xxi
\( J'' \)  Diffusion species mass flux

\( k \)  Dummy constants

\( k_B \)  Boltzmann constant

\( k_{cav} \)  Modified isentropic cavitation model parameter

\( k_f, k_r \)  Forward or reverse chemical reaction rate constant

\( K \)  Dummy constants

\( K_c \)  Concentration equilibrium constant

\( K_n \)  Knudsen number

\( K_p, K_u \)  AUSM dissipation parameters

\( l \)  Length

\( L_p \)  Laplace number

\( L \)  Characteristic wave strength

\( \mathbf{L} \)  Left eigenvector

\( m \)  RKC damping factor

\( m_1 \)  Monomer mass

\( \dot{m}'' \)  Mass flux

\( \dot{m}''' \)  Volumetric mass production rate due to phase change

\( \mathcal{M} \)  AUSM Mach number functions

\( M \)  Mach number

\( Ma \)  Marangoni number

\( M_w \)  Molecular weight

\( n \)  Burning time diameter exponent or normal direction

\( \mathbf{n} \)  Normal vector

\( \mathbf{n} \)  Normal direction
\( \hat{n}_x, \hat{n}_y \) x- and y-components of the normal vector

\( N \) Number density, Tait EOS exponent, or Number

\( N_1 \) Number density of nucleation monomers

\( N_{Av} \) Avogadro’s number

\( N_d \) Number of downstream points for in the WENO stencil

\( N_g \) Number of gaseous chemical species

\( N_l \) Number of chemical species in liquid phase

\( N_{\text{phase}} \) Number of phases

\( N_R \) Number of chemical reactions

\( N_{RS} \) Number of interfacial Riemann Solutions

\( Nu \) Nusselt number

\( N_u \) Number of upstream points in the WENO stencil

\( p \) AUSM pressure vector

\( p \) Pressure

\( p_{\text{cav}} \) Cavitation pressure

\( p_{gl} \) Modified Schmidt cavitation model parameter

\( p_{\text{sat}} \) Saturated vapor pressure

\( P \) Primitive variable vector

\( P \) AUSM pressure function

\( P \) Interpolation polynomial

\( Re_{\text{cell}} \) Cell Peclet number, \( Re_{\text{cell}} = u \Delta x / D \)

\( Pr \) Prandtl number

\( q \) Net reaction rate of progress

\( q_x, q_y \) Heat flux in x- and y-directions

xxiii
\( \dot{q} \)  Heat flux normal to interface

\( q \)  Diffusion heat flux

\( Q \)  Generic variable

\( \mathbf{Q} \)  Generic solution vector

\( Q''' \)  Volumetric rate of heat generation

\( r \)  Radius, MUSCL slope ratio, AMR refinement ratio, or number of points in WENO candidate stencils

\( r_{\text{curv}} \)  Radius of curvature

\( r_b \)  Regression rate

\( r_{\text{nuc}} \)  Rate of nucleation

\( R \)  Gas constant or bubble radius

\( R_u \)  Universal gas constant

\( Re_d \)  Reynolds number based on diameter \( Re_d = \rho ud/\mu \)

\( \mathbf{R} \)  Right eigenvector

\( s \)  Entropy, signal speed

\( s_I \)  Sub-grid interface location

\( S \)  Supersaturation ratio

\( S_L \)  Laminar flame speed

\( \mathbf{S} \)  Source term vector

\( \dot{S} \)  Cavitation rate

\( t \)  Time

\( t_b \)  Droplet life time

\( \mathbf{t} \)  Tangential vector

\( \hat{t} \)  Tangential direction
\( T \)  Temperature or Chebyshev polynomial

\( T_g^g, T_r^g \)  Ghost and real gas temperature

\( T_g^l, T_r^l \)  Ghost and real liquid temperature

\( u \)  Velocity component in x-direction, velocity normal to the interface, or Stockmayer potential

\( u_g^g, u_r^g \)  Ghost and real gas velocity components in x-direction

\( u_g^l, u_r^l \)  Ghost and real liquid velocity components in x-direction

\( u_n \)  Normal velocity

\( \bar{u} \)  Roe averaged velocity

\( \mathbf{U} \)  Conserved variable vector

\( \mathbf{U}' \)  Faux conserved variable vector

\( v \)  Velocity component in y-direction

\( v_1 \)  Monomer volume

\( v_g^g, v_r^g \)  Ghost and real gas velocity components in y-direction

\( v_g^l, v_r^l \)  Ghost and real liquid velocity components in y-direction

\( \mathbf{v} \)  Velocity vector

\( V \)  Primitive function

\( V_{ij} \)  Volume of cell \( ij \)

\( \mathbf{V} \)  Diffusion velocity or primitive variable vector

\( w \)  Velocity component in z-direction

\( \dot{W}^{mm} \)  Interfacial work

\( \text{We} \)  Weber number

\( \mathbf{W} \)  Double flux frozen variable vector

\( x \)  X or axial position
\( \mathbf{x} \)  Position vector

\( X \)  Mole fraction

\( y \)  \( Y \) or radial position

\( Y \)  Mass fraction

\( Z \)  Name of chemical species reactant or product for a chemical reaction or rotational relaxation collision number

**Greek Symbols**

\( \alpha \)  Volume fraction, BDF constants, third body efficiencies, polarizability, unnormalized WENO candidate stencil weighting factor, MLP slope limiter factor, or weighting factor for rotated Riemann solver

\( \alpha_{\text{sun}} \)  Grid refinement parameter

\( \alpha_T \)  Coefficient of thermal expansion

\( \beta \)  RKC stability boundary, inner tube radius for FLLS, Arrhenius temperature exponent, or second viscosity

\( \beta_0 \)  Backwards differentiation parameter

\( \gamma \)  Specific heat ratio or sticking coefficient

\( \tilde{\gamma} \)  RKC parameter

\( \delta \)  Smeared Dirac delta function

\( \Delta p_s \)  Pressure tolerance for shock wave sensor

\( \Delta x \)  Grid spacing

\( \Delta t \)  Time step size

\( \Delta \tau \)  Pseudo time step size

\( \epsilon \)  Well depth or generic small parameter

\( \epsilon_{\text{deref}}, \epsilon_{\text{ref}} \)  Thresholds for grid derefinement and refinement

\( \epsilon_{\text{rot}} \)  Tolerance for activation of the Rotated Riemann Solver
\( \epsilon_s \) Smoothness tolerance
\( \zeta \) Outer tube radius for the fast local level set method
\( \eta \) Kolmogorov scale or coordinate system selector
\( \theta \) Interface sub-cell position factor
\( \kappa \) Volume viscosity
\( \kappa_c \) Curvature
\( \kappa_T \) Isothermal compressibility
\( \lambda \) Mean free path, thermal conductivity, or eigenvalue
\( \mu \) Dynamic viscosity or RKC parameter
\( \mu' = \kappa - 2/3\mu \)
\( \bar{\mu} \) Dipole moment
\( \tilde{\mu} \) RKC parameter
\( \nu \) Stiochiometric reaction coefficients
\( \tilde{\nu} \) RKC parameter
\( \rho \) Density
\( \rho_{gc}, \rho_{tc} \) Modified Schmidt cavitation model parameters
\( \rho_{gs}, \rho_{ls} \) Modified isentropic cavitation model parameters
\( \sigma \) Deviatoric stress tensor, molecular collision diameter, spectral radius, or AUSM dissipation parameter
\( \bar{\sigma} \) Accommodation coefficient
\( \sigma_t \) Surface tension
\( \sigma_{nn} \) Deviatoric interfacial normal stress in the normal direction
\( \sigma_{nt} \) Interfacial shear stress
\( \sigma_{tt} \) Deviatoric interfacial normal stress in the tangential direction
\( \tau \) Characteristic or pseudo time
\( \phi \) Signed distance function, slope limiter, or equivalence ratio
\( \chi \) Dissipation parameter for local Lax-Friedrichs flux
\( \chi_{\text{cav}} \) Cavitation model parameter
\( \psi \) Advected quantity for AUSM scheme or dummy variable
\( \omega \) RKC parameters or WENO candidate stencil weighting factor
\( \dot{\omega}_i^{'''} \) Volumetric mass production of species \( i \)
\( \dot{\omega}_i^{''} \) Mass flux of species \( i \) at interface
\( \Omega \) Collision integral or domain

**Subscripts**

0 Initial or reference value
1/2 Interface quantity
accr Accretion
b Bubble, boundary, or burn time
c Condensed phase particles or corrected
cav Cavitation
chem Chemical
coll Collision
cont Continuous phase
cor Corrected
d Direction or number of downstream cells in WENO stencil
diff Diffusion
eff Effective
evap  Evaporation
f  Flame
face  Cell face
g  Gas phase or ghost variable
H  Heterogeneous
i  Species or grid point index in x-direction
init  Initial
I  Interface
j  Grid point index in y-direction
k  Phase or WENO candidate stencil index
l  Liquid phase variable
loc  Location
L  Left edge interpolated value
m  Liquid/vapor mixture
mix  Multicomponent mixture
mfp  Mean free path
n  Normal direction
nuc  Nucleation
p  Particle
r  Real variable
rel  Relative
rot  Rotational
R  Right edge interpolated value
s  Surface

xxix
Sat Saturation
st Stoichiometric
t Tangential direction
tot Total
trans Translational
u Number of upstream grid points in WENO stencil
v Vapor
vib Vibrational
vn Condition in von Neumann spike

Superscripts
* Critical value, reduced value, or starred state for Riemann problem
g Gas variable
l Liquid variable
m Property table interval
n Time level
r Number of grid points for WENO candidate stencils
T Transpose

Operators
[ψ] Interface jump, ψg − ψl
∇s Surface gradient, ∇ − ěดน/ดน
 Hacker Hyperbolic PDE integrator
≌ Parabolic PDE integrator
S Source term PDE integrator
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1.1 Uses of Aluminum Particles

Because aluminum is an energetic fuel additive for solid propellants and solid fuels in different propulsion systems, and because of the effectiveness of particle damping in suppressing combustion instabilities in rocket motors, aluminum particles have been widely employed in combustion applications. The importance of aluminum in combustion systems has led to a large number of experimental studies of aluminum combustion, but far fewer theoretical modeling studies.

A comparison of the gravimetric and volumetric heat of oxidation for various metallic fuels is shown in Figure 1.1. While both boron and beryllium release more energy than Al, boron is extremely difficult to ignite and the products of beryllium oxidation are very toxic [1]. Titanium and tungsten have comparable heating values per unit volume to Al, but have far lower heating values per unit mass. Because of its high amount of heat release per unit volume and per unit mass, aluminum has been one of the most used and most studied energetic additives to solid propellants and explosives.

In propulsion applications aluminum particles are mixed with the solid propellant. When the solid propellant burns the surface recedes exposing molten aluminum particles. The exposed aluminum particles are then entrained by the strong convective flow of solid propellant...
combustion products where they burn in the high temperature \((T \approx 3500 \text{ K})\) and high pressure \((p \approx 650 \text{ psi})\) environment. One of the key advantages of metal fuels is that they react readily with typical hydrocarbon combustion products such as \(\text{CO}_2\) or \(\text{H}_2\text{O}\) in addition to oxygen. The primary aluminum combustion product of aluminum combustion is condensed-phase aluminum oxide (often called alumina), \(\text{Al}_2\text{O}_3\). When the Al oxidizers are water vapor and carbon dioxide, alumina is formed by stripping the oxygen atoms from the oxidizers forming a fuel rich mixture of \(\text{H}_2\) and \(\text{CO}\). So not only does aluminum add energy to the system, it also decreases the molecular weight of the gas-phase propellant products. Both of these effects increase the overall efficiency of the propulsion system.

Another area that utilizes aluminum particles is thermobaric explosives (TBX). A TBX is a heterogeneous aluminized explosive where the aluminum particles are either mixed with the high explosive (HEX) material itself, or the particles are placed in a cylindrical (or spherical) shell between the explosive casing and the HEX material. The processes of a TBX detonation proceeds as follows \([2, 3]\) and are shown in Figure 1.2. First, the HEX charge is detonated, producing a strong shock wave and contact surface as shown in Figure 1.2b. The high velocity
Figure 1.2: Sequence of events during the detonation of a TBX charge.

gas behind the shock and contact surface accelerates away from the center of the detonation as shown Figure 1.2c. As time continues, the smaller aluminum particles absorb enough energy from the high temperature detonation products and ignite. These smaller ignited particles burn anaerobically with CO$_2$ and H$_2$O in the HEX detonation products behind the contact surface. As the processes continues on, the larger Al particles ignite, producing more heat, H$_2$, and CO from the HEX detonation products. As the particles accelerate, some of them move outside of the contact surface and continue to react in the shock-heated air. A side effect of a cylindrical or spherical explosive is that as the primary shock moves radially outward it weakens and the post-detonation gases expand, limiting the time that the largest particles have to ignite. Some of the larger particles achieve enough momentum
Figure 1.3: Calculated density on an x-t diagram for the spherical Riemann problem with an initial pressure and temperature of 100 atm and 3000 K in the 0.5 m blast using the MPWENO9 algorithm described in Appendix B and the local Lax-Friedrichs flux vector splitting approach described in Chapter 3.

to outrace the primary shock and continue to react aerobically with the ambient air. As the primary shock moves outwards and weakens, a rarefaction wave propagates towards the center of the blast and strengthens due to focusing effects from the radial symmetry. The inward motion of the rarefaction wave over-expands the detonation products when the TBX charge is either cylindrical and spherical, producing a weaker secondary shock wave that moves radially inward as shown in Figure 1.3. The secondary shock is much weaker but may introduce hydrodynamic instabilities, such as the Richtmyer-Meshkov instability, which aid mixing of fuel particles that remain near the center of the blast.

If the TBX charge is detonated in the open, the largest aluminum particles may not absorb enough energy to ignite, but the smallest aluminum particles will ignite and release energy quickly enough to enhance the strength of the blast. An interesting situation occurs if the charge is detonated in a closed room. In this case, the room—assuming it survives the blast—provides partial confinement to the explosive, limiting the expansion of the detonation
products and giving more time for the aluminum particles to ignite. The primary shock wave eventually reflects off the walls, giving the aluminum particles a greater chance to ignite in the double-shock heated air as shown in Figure 1.2d. When the reflected shock waves interact with the contact surface, Richtmyer-Meshkov (RM) instabilities [4] are introduced. The RM instability mixes fuel species produced from aluminum particles reacting with the HEX detonation products and the double shock heated air. The air and fuel species react and release even more energy. Even though this extra energy release is too late for blast enhancement purposes, it works very well for applications that require a large amount of heat to be released in a short amount of time.

The primary goal of this work is to obtain detailed understanding of how shock waves interact with burning Al droplets. As described above, Al particles burn in a variety of conditions for TBX applications depending on where and when they are studied. The pressure and temperature can be extremely high if the study includes the very early phases of the TBX detonation where the particles are initially entrained and burn in the HEX detonation products. If later times are chosen and the distance is far away from the blast center, the pressure and temperature will be nearly atmospheric and the aluminum particles that are reacting with air may be impacted by a shock wave. The physics of either case are complicated; however, simulating the particles that stay inside the contact surface requires complex Al/O/H/C chemistry and a real gas equation of state for multi-component mixtures. Since computing real gas flows without chemical reactions or particle dynamics is still a very difficult research area, emphasis is placed on Al droplets that react in air and interact with a reflected shock wave. This allows the ideal gas law to be used, greatly simplifying the model.

Before the combustion of aluminum droplets is discussed, some basic results of droplet vaporization and combustion are reviewed.

1.2 Overview of Droplet Vaporization and Combustion

The fundamental theory of droplet vaporization can be found in many sources [5–9]. If a simple mass balance on an evaporating (or condensing) droplet is considered, we find that

\[
\frac{dr_p}{dt} = -\frac{\dot{m}_{\text{evap}}}{\rho_l},
\]

(1.1)

where \( r_p \) is the droplet radius, \( \dot{m}_{\text{evap}} \) is the mass flux leaving the liquid surface, and \( \rho_l \) is the density of the droplet.
The evaporation of a liquid is a two-step process. First vapor molecules are generated at the surface, then vapor molecules are transported away from the surface by a combination of diffusion and the blowing velocity. The regression rate of the droplet is determined by the slower of these two processes. In the transport limited (often called diffusion limited) case, the surface mass flux is:

\[
\dot{m}_{\text{evap}}'' = \frac{\rho_g D}{r_p} \ln(1 + B),
\]

where \(D\) is the mass diffusivity for the vapor and \(B\) is the Spalding transfer number:

\[
B \equiv \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}}.
\]

\(Y_{v,s}\) is the vapor mass fraction at the droplet surface and \(Y_{v,\infty}\) is the vapor mass fraction far away from the droplet. The vapor mass fraction at the droplet surface can either be determined using the Clausius-Clapeyron relation or from experimental measurements of saturation vapor pressure as a function of temperature. Substituting Eq. (1.2) into Eq. (1.1) and integrating gives:

\[
r_p^2 = r_{p,0}^2 - \frac{2\rho_g D}{\rho_l} \ln(1 + B)t,
\]

which is the \(d^2\) law of droplet vaporization. This law is valid for many practical applications; however, it neglects the vapor generation process.

As the droplet diameter decreases, the diffusion-limited evaporation rate increases without bound. When the droplet size is very small—typically on the micrometer scale or less—the rate that the surface can generate vapor becomes comparable to the rate of transport from the surface. If the size of the droplet is decreased even further the regression of the droplet is limited by the generation rate. Using kinetic theory, Schrage [10] derived the vaporization rate of a planar surface as:

\[
\dot{m}_{\text{evap}}'' = \frac{2c}{2 - c} \sqrt{\frac{M_w}{2\pi R_u}} \left[ \frac{p_{\text{sat}}}{\sqrt{T_{p,s}}} - \frac{p_v}{\sqrt{T_{v,s}}} \right],
\]

where \(c\) is the condensation coefficient, \(M_w\) is the molecular weight of the evaporating vapor, \(R_u\) is the universal gas constant, \(p_{\text{sat}}\) is the saturated vapor pressure, \(p_v\) is the partial pressure of vapor at the surface, and \(T_p\) and \(T_v\) are temperatures of the droplet and vapor at the
surface, respectively. If we substitute this expression into Eq. (1.1), we get:

\[ r_p = r_{p,0} - \frac{2c}{2 - c} \sqrt{\frac{M_w}{2\pi R_u \left( \sqrt{T_{p,s}} - \sqrt{T_{v,s}} \right)}} t. \] (1.6)

Thus, if the vaporization of a droplet is limited by kinetic theory (or just kinetic limited) the \(d^2\) law transitions to a \(d^1\) law.

The droplet radius where the surface generation rate equals the rate of transport from the surface can calculated by equating Eqs. (1.2) and (1.5) and solving for \(r_p\). A plot of the droplet radius when the rate of vapor transport is equal to the vapor generation rate is shown in Figure 1.4. Above this radius the vaporization rate is limited by transport from the surface. Below this radius the vaporization rate is limited by the rate of vapor generation. The transition between diffusion and kinetic theory limited vaporization of an Al droplet can be anywhere from 30 nm to 100 \(\mu\)m depending on the pressure and temperature of the particle and the condensation coefficient assumed. When equating the diffusion limited and kinetic limited vaporization rates, it was assumed that the vapor mass fraction far from the surface was zero, the vapor and liquid surface temperatures were equal, and the condensation coefficient was unity. The saturation pressure and the binary diffusion coefficient between Al and \(O_2\) were calculated using the procedures given in Appendix A.

For diffusion limited droplet combustion, the evaporated fuel and oxidizer mix and react completely in an infinitesimally thin flame sheet (indicated by a thin orange line in Figure 1.5) some distance away from the surface of the droplet as shown in the diffusion limited line Figure 1.5. The vaporization rate of a burning droplet is similar to the non-reacting case, except that the Spalding transfer number is larger:

\[ B \equiv \left( \frac{F}{O} \right)_{st} Y_{O,\infty} + Y_{v,s} \left( 1 - Y_{v,s} \right), \] (1.7)

where \((F/O)_{st}\) is the stoichiometric mass fuel to oxidizer ratio.

If the droplet diameter is small, the diffusion rate may exceed the rate at which gas-phase chemical reactions occur. The Damköhler number, \(Da\), is defined as the ratio of the characteristic diffusion time to the characteristic chemical reaction time:

\[ Da \equiv \frac{\tau_{\text{diff}}}{\tau_{\text{chem}}} \approx \left( ar_p \right)^2 \frac{\tau_{\text{chem}}}{D}, \] (1.8)
Figure 1.4: Al droplet radius, $r_p$, where the rate of vapor transport from the surface equals the kinetic rate of vapor production (a) as a function of particle temperature at various pressures with $c = 1$ and (b) at various condensation coefficients at atmospheric pressure.

where $a$ represents the number of particle radii that an oxygen molecule must travel to reach the particle surface. For a stoichiometric Al vapor/air mixture, the gas phase chemical reaction time, $\tau_{\text{chem}}$, is on the order of $1 \mu s$ [11]. Taking $a$ to be five and using the Al-O$_2$ binary diffusion coefficient at $T = 2000$ K, we find that the particle radius where the diffusion time and the chemical reaction time are equal is around $4.5 \mu m$.

The flame sheet, which is infinitesimally thin in the diffusion limited case (i.e., infinite Damköhler number), starts to thicken (indicated by the thick orange line in Figure 1.5) and decreases in strength as the Damköhler number approaches unity as shown by the transitional line in Figure 1.5. Situations where both diffusion and chemical kinetics are important are called the transitional regime. Oxidizers, which are reacted completely at the flame sheet in the diffusion limited case, may reach the particle surface in the transitional regime and thus, may attack the surface directly by heterogeneous chemical reactions.

If the Damköhler number approaches zero the gaseous diffusion flame structure disappears completely, and chemical reactions occur on the surface or immediately above it. This extreme is shown on the kinetic limited line of Figure 1.5.
Figure 1.5: Qualitative flame structures of diffusion limited, transitional, and kinetic-limited droplet combustion.

1.3 Al Particle Combustion

1.3.1 General Al Combustion

Now that some of the basic theory of droplet combustion and the meaning of diffusion, kinetic, and transitional regimes of droplet combustion have been explained, a brief discussion of Al particle combustion can proceed.

Despite the advantages of using Al particles in propulsion systems and thermobaric explosives, aluminum has its challenges to be effectively utilized. Al particles have a protective oxide layer of alumina, Al$_2$O$_3$, which serves as a barrier to ignition and has a thickness on the order of 8 nm for 100 nm diameter particles [12]. In many practical combustion situations aluminum will burn as a molten droplet after the aluminum oxide layer is removed. At atmospheric pressure alumina melts at 2327 K [13], which gives an upper limit on the ignition temperature. Measurements of the ignition temperature for traditionally sized Al particles ($d_p > 20 \mu$m) can lie anywhere between 1900 and 2300 K [14], indicating that Al ignition may occur due to oxide shell cracking as well as melting.

In propulsion applications the deflagration of the propellant exposes Al particles in a rather gentle process in comparison to the detonation of a TBX. The detonation of an explosive charge is a violent process, with pressures and temperatures reaching 10 GPa and 3500 K or more. In these extreme environments even solid metal particles cannot be treated as rigid bodies and behave almost like a fluid [15, 16]. Thus, the particles are massively de-
formed which destroys the oxide layer. Similar conclusions were obtained from experimental measurements by Gilev and Anisichkin [17]. During the passage of the detonation wave, the temperature of the Al particles can reach 900 K due to compression [16].

When aluminum burns its main combustion product is condensed-phase alumina. Most of the alumina is formed in the flame sheet and is advected downstream of the Al droplet in a smoke trail as shown in Figure 1.6. Not all of the nano-sized aluminum oxide droplets are advected downstream of the droplet; some may deposit on the liquid aluminum and grow a cap of liquid aluminum oxide since liquid Al and liquid alumina are immiscible [19]. The
Figure 1.7: Flame temperatures for stoichiometric mixtures of Al/O\textsubscript{2} versus (a) initial reactant temperature at atmospheric pressure and (b) as a function of pressure.

The presence of this oxide cap—initially formed by the melting of the alumina shell—blocks a portion of the droplet from vaporizing or reacting with the oxidizer, reducing the $d^2$ law for the combustion of large aluminum droplets to a $d^{1.8}$ or $d^{1.5}$ law [14].

One peculiarity of alumina is that it does not exist in the gas phase. It is generally accepted that alumina dissociates into aluminum sub-oxides such as AlO, Al\textsubscript{2}O, and Al\textsubscript{2}O\textsubscript{2} and O before it vaporizes. The dissociation of alumina is pivotal in determining the flame temperature, $T_f$, of Al [20]. As shown in Figure 1.7a, the dissociation of liquid alumina keeps the flame temperature (calculated using NASA-Lewis CEA [21]) between 3910 and 3940 K for initial reactant temperatures ranging from 273 K to 4500 K. The nearly constant flame temperature of Al is in stark contrast with typical hydrocarbons. Calculations of stoichiometric hydrogen-oxygen combustion reveal that the flame temperature increases from 786 to 2358 K when the initial temperature of the reactants is increased from 273 to 2000 K. The near constant Al flame temperature at a given pressure has prompted some researchers [22–24] to use ad hoc methods to impose this nearly constant flame temperature by changing alumina dissociation/condensation rates depending on temperature.

Even though the flame temperature of Al is almost independent of the reactant temperature, it is strongly dependent on pressure. If one of the alumina dissociation reactions of Huang et al. [11] is examined, say Al\textsubscript{2}O\textsubscript{3} ⇌ AlO + AlO\textsubscript{2}, and Le Chatelier’s principle is applied, it can be concluded that as pressure increases the equilibrium concentration will
tend to favor more alumina over the dissociation products. Since the flame temperature of Al is predominantly tied to alumina concentration, the flame temperature tends to increase with increasing pressure. This effect is shown in Figure 1.7b. The boiling point [calculated using Eq. (A.82)] of A will exceed the flame temperature of stoichiometric Al/air mixtures at about 1000 psia. When this occurs the evaporation mass flux is severely reduced, allowing some oxidizers to reach the particle surface and attack it heterogeneously no matter the rate of diffusion or particle size.

1.3.2 Experimental Al Particle Combustion Results

In a survey of many experimental studies on aluminum particle combustion, Beckstead [14] found that burning times of Al particles are in reasonable agreement with a $d^n$ law where $n = 1.5$ to 1.8. His findings also indicate that water vapor and carbon dioxide are 60% and 22% as effective as oxygen at burning aluminum, respectively. As predicted by diffusion limited theory, Beckstead found that the burning time of an aluminum droplet is weakly dependent on both ambient temperature and pressure. His overall correlation on aluminum burning times, $t_b$, is:

$$t_b(\text{ms}) = \frac{a d_p (\mu \text{m})^n}{X_{\text{eff}} P \text{(atm)}^{0.1} T_0 \text{(K)}^{0.2}},$$

(1.9)

where $X_{\text{eff}}$ is the effective oxidizer concentration,

$$X_{\text{eff}} = X_{O_2} + 0.6 X_{H_2O} + 0.22 X_{CO_2},$$

(1.10)

and $X_i$ is the mole fraction of species $i$. The parameters $a$ and $n$ are $a = 0.0244$ if $n = 1.5$ or $a = 0.00735$ if $n = 1.8$. As mentioned earlier, the reduction of the diameter exponent from two to either 1.5 or 1.8 is largely caused by the formation of an aluminum oxide lobe on the surface of the aluminum particle during combustion.

Using planar laser induced fluorescence (PLIF) on falling Al droplets, Bucher et al. [25] identified some of the chemical species present in the immediate vicinity of aluminum droplets burning in various gases and gas mixtures including CO$_2$, N$_2$O, CO, and O$_2$, N$_2$, and Ar at atmospheric pressure. They identified that aluminum monoxide, AlO, is a primary gas-phase product species under all conditions tested. Clearly AlO chemistry must be considered in both oxygen-rich environments and typical solid propellant or HEX product environments.
Sarou-Kanian et al. [26, 27] burned large aluminum particles (on the order of 3 mm) in carbon dioxide using an aerodynamic levitator. Their findings indicated that carbon can deposit on the surface of the particle in CO$_2$ gas environments, suppressing the rate of aluminum vaporization and heterogeneous reactions. Sarou-Kanian et al. [26] found that small amounts of water vapor or hydrogen in CO$_2$ gas mixtures can cause the oxide shell to recede; however, in dry CO$_2$ the oxide shell did not recede. It was also observed that carbon can dissolve into the Al droplet, eventually forming a carbon shell on the molten Al droplet surface after the liquid is saturated with carbon, which can prevent further oxidation of the Al particle. When burnt particles were cross-sectioned and examined using X-ray diffraction techniques, it was discovered that Al, Al$_2$O$_3$, Al$_4$C$_3$, and Al$_4$O$_4$C were present in the particle interior, indicating that carbon dissolution occurred during combustion. While the results of these two studies are scientifically meaningful, carbon dissolution is not considered in this work since the of CO$_2$ is relatively low in typical rocket or explosive environments.

All the experimental work discussed thus far has focused on larger Al particles that are diffusion limited. Bazyn et al. [28] studied the combustion of 10 µm-sized aluminum particles in the reflected region of a shock tube. They found that carbon dioxide is twice as effective as water vapor in burning these smaller Al particles, which is completely opposite of Beckstead’s findings [14]. They also found pressure exponents (i.e., $t_b \sim p^n$) of -0.9, 0.3, and 0.2 for O$_2$, CO$_2$, and H$_2$O, respectively on the particle burning time. The strong pressure exponent for oxygen is indicative of chemical kinetic-controlled combustion mechanisms, whereas the low pressure exponent values for carbon dioxide and water vapor are indicative of diffusion controlled combustion mechanisms.

Bazyn et al. [29] performed shock tube measurements on 40-µm diameter and smaller aluminum particles. They found that the transition from diffusion- to kinetic-controlled combustion begins at around 10 µm at 8.5 atm for particles burning in O$_2$/Ar mixtures, which is in the size range predicted by both kinetic theory. For particles burning in CO$_2$/Ar mixtures, they found that the beginning of the transitional regime begins when the diameter of Al particles is around 40 µm. They also found that diameter exponents on the burning times of transitional Al particles (i.e., $t_b \sim d^n$) are between 1.09 and 1.15 when CO$_2$ is the main oxidizing species and between 0.68 and 0.69 when O$_2$ is the main oxidizing species. These results directly indicate that the $d^2$ law is not valid for smaller Al particles.

Bazyn et al. [29] measured the flame temperature of burning Al particles using AlO spectroscopy and particle temperature using optical pyrometry. Their findings indicated that
Table 1.1: Coefficients used for Eq. (1.11).

<table>
<thead>
<tr>
<th>Oxidizer</th>
<th>( a_0 (\mu s/\mu m^{n_i}) )</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{O}_2 )</td>
<td>200</td>
<td>0.5</td>
<td>-0.5</td>
</tr>
<tr>
<td>( \text{CO}_2 )</td>
<td>500</td>
<td>0.6</td>
<td>0.3</td>
</tr>
<tr>
<td>( \text{H}_2\text{O} )</td>
<td>86</td>
<td>-1.7</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Al particles with a diameter greater than 20 \( \mu m \) have a flame temperature above the boiling temperature of the Al particle, indicative of a diffusion flame structure. When the particle diameter was decreased to 10 \( \mu m \) they observed that the flame temperature approached the Al boiling point, which is indicative of chemical kinetic limited combustion.

Lynch et al. [30] correlated shock tube data on Al particle burning times with diameters ranging from 3 to 11 \( \mu m \). Their correlation is given by:

\[
t_{b,i}(\mu s) = a_{0,i} X_i^{a_{1,i}} \left( \frac{p}{p_0} \right)^{a_{2,i}} d_p(\mu m)^{n_i},
\]

\[
n_i = 2 \exp(-4.3 X_i) \left( \frac{p}{p_0} \right)^{-0.3},
\]

\[
t_{b,\text{mix}}(\mu s) = \left[ \frac{1}{t_{b,O_2}} + \frac{1}{t_{b,\text{CO}_2}} + \frac{1}{t_{b,\text{H}_2\text{O}}} \right]^{-1},
\]

where \( p_0 = 8.5 \) atm and the other coefficients used for Eq. (1.11) are given in Table 1.1.

Bazyn et al. [29, 31] also studied the combustion of 80 nm diameter Al particles in their shock tube apparatus. In sharp contrast to diffusion limited or even transitional Al particle combustion, the burning times of nano-aluminum is heavily dependent on the ambient temperature, following an Arrhenius-like exponential form. Parr et al. [32] obtained similar temperature dependence for nano-aluminum burning times up to diameters of 200 nm using a Hencken burner apparatus. Parr et al. [32] also found stable ignition temperatures as low as 1200 K for nano-Al, while the ignition temperature of micron Al is near the alumina melting temperature. A detailed discussion of nano-Al combustion is beyond the scope of this work, but is thoroughly discussed in Puri [33].

All of the burning time correlations were developed for use in propulsion applications where the Al particles are essentially flow-borne. No correlations for Al particle combustion burning times could be found in the open literature that are suitable for blast applications where they may be exposed to high slip velocities and shock waves. Most studies prior to
this work did not examine the interaction between burning Al particles and shock waves; the shock tube was used to provide a controllable environment to study the combustion of Al particles in a quiescent environment. Thus, current Al burning time correlations may need to be modified for use in applications with shock waves and high velocity slip.

Recently Tanguay et al. [34] performed Al particle combustion experiments of Al particles burning in highly convective environments using a detonation tube. Their results showed that Al particles tend to burn in a kinetically limited manner when they are accelerated in highly convective flows.

Aluminum combustion is not only of interest to energetics community, but also to the safety community as well. Many air separation plants use aluminum tubing and heat exchangers that can flow high-pressure LOx or GOx. Steinberg et al. [19] studied the promoted combustion of Al rods in high pressure GOx, and used a simplified model to estimate the heterogeneous regression rate of the aluminum rod assuming a Langmuir-Hinshelwood [35] expression. They found that heterogeneous reaction rate of Al with high-pressure GOx can be expressed by:

\[
\dot{m}_{Al}'' \text{(g/m}^2\text{s)} = \frac{0.102p_{O_2}(\text{MPa})}{1 + 0.186p_{O_2}(\text{MPa})}.
\]  

(1.14)

This is the only heterogeneous reaction rate of Al that could be found at this time which is directly usable in a CFD calculation. In follow-up work, Wilson and Stoltzfus [36] suggested a different form for the heterogeneous reaction rate of Al, \( \dot{m}_{Al}'' = kK\sqrt{p_{O_2}}/(1 + K\sqrt{p_{O_2}}) \). Unfortunately they did not give the constants to their modified heterogeneous burning rate.

Wilson and Stoltzfus [36] also hypothesized that the burning of Al slabs can proceed in one of two ways. If the flame temperature is lower than the alumina melting point (which is slightly porous) the oxidation of aluminum proceeds by chemisorption of oxygen onto the solid alumina surface and dissociating into oxygen atoms. The oxygen atoms then diffuse through the porous alumina coating and attack the liquid Al surface, thickening the oxide coating. If the alumina shell is molten, internal circulation within the liquid metal and alumina expose fresh liquid Al that can react heterogeneously with oxidizers or vaporize. It is interesting to note that the low temperature version of Wilson and Stoltzfus’s aluminum sheet oxidation mechanism is very similar to some hypothetical mechanisms for the combustion of nano-sized Al particles [37].
1.3.3 Al Particle Combustion Models

In contrast to the plethora of experimental work, far fewer detailed modeling studies of Al particle combustion are available. One of the first models was developed by King [38], which is similar to one dimensional droplet combustion models presented in many texts [5, 6]. Reactions were allowed to take place only at an infinitesimally thin sheet where alumina condenses and fuel (aluminum vapor) only exists in the region between the particle and the condensation sheet. In addition to evaporation, heterogeneous surface reactions were also considered in this model: \(2\text{Al(l)} + \text{CO}_2 \rightleftharpoons \text{Al}_2\text{O} + \text{CO}\) and \(\text{Al(l)} + \text{AlO} \rightleftharpoons \text{Al}_2\text{O}\). Even though surface reactions were used, the rate expressions for these reactions were not (and likely still not) known and King was forced to make the assumption that surface reactions are infinitely fast.

Later Beckstead et al. [22] and Washburn et al. [23] developed a two-dimensional model of aluminum particle combustion. The most notable feature of their model was alumina condensation, which was treated using homogeneous nucleation theory. Modeling alumina condensation is problematic since it does not exist in the gas phase since it dissociates before it vaporizes. Thus, it is impossible to measure or even rigorously define saturation pressure. To overcome this Beckstead et al. [22] defined the degree of supersaturation for alumina as:

\[
S = 1 + \frac{P_{\text{AlO}} + P_{\text{AlO}_2} + P_{\text{Al}_2\text{O}}}{P_{\text{Al}}},
\]  

(1.15)

They made the assumption that the net condensation reaction was a two-step process, with the first step being the formation of gaseous alumina followed by nucleation of alumina droplets. This mechanism proceeds by: \(aA + bB \rightarrow \text{Al}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3(l)\), where A and B refer to gas phase reactants that may form alumina such as AlO and \(\text{O}_2\) or \(\text{Al}_2\text{O}\) and \(\text{CO}_2\). They derived the net condensation rate for each reaction involving alumina as:

\[
\dot{\omega}_{\text{cond}} = K r_{\text{nuc}} [A]^a [B]^b,
\]

(1.16)

where \(r_{\text{nuc}}\) is the rate of the nucleation step, \([A]\) and \([B]\) refer the concentrations of species A and B, and \(K\) is an empirical constant which is the same for all alumina condensation reactions. In a move that happens far more often than it should, the authors [22, 23] never mention what \(K\) value they used in their work. They also assumed that alumina deposits
uniformly onto the particle and coalesces into an oxide cap, which blocks certain areas on
the droplet surface from vaporizing.

In their earlier work, Beckstead et al. [22] forced an upper limit on the gas-phase flame
temperature, \( T_f \), to be:

\[
T_f(\text{K}) = \frac{1}{0.000250501 - 14.132 \times 10^{-6} \ln p(\text{atm})},
\]

by using a function to dissociate some alumina if the temperature is greater than the flame
temperature. They also adopted the infinitely fast surface reactions of King [38]. Their
calculated burning times agree well with experimental data, and their predicted \( d^n \) law
exponent is 1.9 for larger particles and 1.2 for smaller particles.

The model of Beckstead et al. [22] was extended [23] to include the latest detailed gas
phase chemical reactions. The results of this model correctly calculated a single aluminum
particle reacting with steam and produced some of the empirical results for Al droplet com-
bustion, namely that the burning time of large particles is relatively independent of pressure,
while the burning time of particles in the transitional regime is a function of pressure.

Recently, Gallier et al. [39] developed a model to study the effect of acoustic waves on
burning Al droplets. They assumed that the droplet was at the boiling point and the alumina
condensation reaction is: \( \text{O}_2 + 4\text{AlO} \rightarrow 2\text{Al}_2\text{O}_3(l) \). Their calculations produced the proper
diffusion flame structure and burning time. They also found that at low Reynolds numbers,
the effect of convection on the burning rate of the Al droplets can be computed using the
Ranz-Marshall correlation [40] with a fair amount of accuracy.

1.3.4 Items to Consider when Shock Waves Interact with Burning Al Droplets

To date, all models of Al particle combustion assume that the droplet is a rigid sphere.
The emphasis of prior models is for propulsion applications where convection on the droplet
surface is weak due to entrainment. None of these models address how Al droplets burn
in environments containing shock waves. When a shock wave impacts a liquid droplet the
pressure and high-speed flow behind the shock wave can possibly deform and/or possibly
strip the liquid off the droplet surface [41] depending on the Weber and the Reynolds numbers
of the droplet. In this work the Weber number is defined as:

\[
\text{We} = \frac{\rho g v_{\text{rel}}^2 d}{\sigma_t},
\]
where $\sigma_t$ is the surface tension of the droplet. According to Borisov [42] the breakup of a droplet can be classified into three regimes depending on the Weber number of the droplet and $WeRe_d^{-1/2}$. If $8 \leq We \leq 40$ and $0.2 \leq WeRe_d^{-1/2} \leq 1.6$ the droplet deforms into a parachute shape or a claviform shape as shown in Figure 1.8. When $20 \leq We \leq 2 \times 10^4$ and $1 \leq WeRe_d^{-1/2} \leq 20$ the droplet flattens perpendicular to the flow and Rayleigh-Taylor instabilities (RTI) form on the surface of the droplet. The liquid caps of the RTI are sheared off by the high-speed flow and the droplet surface is stripped off, layer-by-layer. An experimental image of this droplet stripping mechanism is shown in Figure 1.9. Although Borisov [42] characterized a regime where the droplet shatters into many smaller droplets instantly if $2 \times 10^3 \leq We \leq 2 \times 10^5$ and $20 \leq WeRe_d^{-1/2} \leq 200$, this catastrophic regime is seldom observed experimentally [43].
Although not well characterized, droplet deformation only occurs if the Weber number is greater than a critical Weber number, $We^*$. If $We < We^*$, the droplet—assuming it was initially spherical—will remain spherical during entrainment. Using the viscosity correlation of liquid Al given in Eq. (A.84) and using Figure 2.25 of Bayvel and Orzechowski [41], $We^* \approx 5$ for this liquid Al droplet. The maximum diameter of an Al droplet that would survive disintegration:

$$d_{max} = \frac{\sigma v^*}{\rho g v_{rel}^2}.$$  \hspace{1cm} (1.19)

Recent advances in multi-fluid computational methods have allowed researchers to calculate the complex interaction of shock waves and compressible liquid droplets [44–47]. These modern methods are not only capable of calculating the complex wave reflections inside the droplet as shown in Figures 1.10 and 1.11, but also capable of predicting large-scale droplet deformation and breakup as shown in Figure 1.12.

Notice that in Figure 1.10 there is a strong interaction of rarefaction waves reflected from the back surface of the droplet at 10 $\mu$s. If strong enough, the interaction of rarefaction waves may cause localized cavitation [44, 46] and may induce spallation of the droplet. Experiments show that when a liquid is subjected to high tensile stresses, bubble nuclei begin to form and grow due to cavitation [48, 49]. A foam-like structure is formed when the cavitation bubbles grow to a very large size. As time continues, the foam structure transitions into dispersed droplets. The formation of cavitation bubbles may cause the droplet to fragment as shown in Figure 1.13.

1.4 Overview of Modeling Interactions Between Shock Waves and Reacting Droplets

In this work a detailed model of the interaction between a shock wave and a reacting droplet was developed. This model focuses on a single droplet and calculates the physicochemical processes of shock waves interacting with burning Al droplets. Examining the combustion of Al droplets in a TBX blast may lead to many diverse situations. Initially, Al particles will be at very high pressures and burn in the TBX detonation products. As time increases, the pressure acting on the Al particles decreases from the outward movement of the blast wave or the inward movement of the rarefaction wave, leading to situations where the Al droplets
Figure 1.10: Internal wave structure of a shock wave interacting with a liquid droplet [44].
can burn in low-pressure detonation products. Particles that outrace the shock wave will react with ambient air and can interact with shock waves that reflect off any nearby walls.

This thesis focuses on larger Al droplets that react with air and interact with a shock wave; simulating Al droplets that outrace the contact surface produced by the detonation of an aluminized HEX charge and are subsequently impacted by a reflected shock wave. A diagram of the computational domain and boundary conditions is shown in Figure 1.14.

In general, solving this problem with the detailed physics described above requires five different phases: gas, condensed-phase alumina droplets, liquid aluminum, liquid alumina, and possibly Al vapor bubbles. Liquid aluminum and liquid alumina are different phases since they are immiscible. Thus, proper simulation of a growing oxide cap requires the addition of a separate liquid alumina phase. Currently, there are not any methods to simulate this large number of compressible phases. Realizing that condensed phase alumina particles are only present since liquid aluminum and liquid alumina are immiscible [19] in the gas phase region and cavitation bubbles are only present in the liquid region, every spatial location will contain two phases at most. Using modern surface capturing methods, the boundary between the gas-phase and liquid-phase regions can be tracked and standard two-phase models can be applied in each region.
Figure 1.12: Computation of shock wave and water droplet interaction showing indicating severe droplet deformation and tearing [47].
1.4.1 Overview of Surface Capturing Methods

It is clear that traditional multiphase methods, which assume that particles are much smaller than the grid spacing, cannot be used in this work since the aim is to capture the interfacial dynamics of a burning Al droplet. Modern interface capturing methods should be used to separate the domain into gas and liquid regions. There are a multitude of techniques for capturing an interface in multiphase flow, including the volume of fluid (VOF) method [50–53], Level Set Method (LSM) [44, 54–57], front tracking (FT) [47], and two-fluid methods [45, 46, 58].

1.4.1.1 Volume of Fluid Method

The VOF method solves the Navier-Stokes equations and tracks a color function that indicates how much of each fluid is in a particular computational cell. The fluid properties in each cell are mixed based on the value of the color function. The main advantage of the
Figure 1.15: Schematic diagram of the dovetail problem for front tracking.

VOF method is that it is conservative through the use of specialized advection algorithms [51, 53] that force the interface to be dispersed over a single cell. A disadvantage of the VOF method is that including effects such as surface tension can be problematic due to the surface curvature being inaccurate [54]. It is possible to show source terms that account for phase change are proportional to the color function gradient magnitude [59]. As the mesh is refined, source terms due to phase change become extremely large since the VOF method keeps the interface contained within one cell. It is also in the author’s experience that standard VOF methods cannot deal with the Stefan (or blowing) velocity at the interface properly. In certain instances the VOF method can assign the blowing velocity to the liquid phase, creating a “tugging” effect that can drag the droplet against the flow. More elaborate and recent attempts seem to have overcome this problem for incompressible flow [60].

1.4.1.2 Front Tracking Methods

Front tracking methods seed the interface with massless Lagrangian particles that move with the surface. The computed shock wave and deforming droplet interaction results of Terashima and Tryggvason [47] shown in Figure 1.12 were obtained with the front tracking method. These methods have the advantage of being accurate but can be difficult to implement, especially in three dimensions [54]. The reason for the difficulty in implementation is that surface topology may change if the surface deforms or moves normal to itself. To capture changes in topology, the connectivity of the Lagrangian particles may have to be changed by cutting, removing, or adding particles. Consider the surface regression of the triangular shape in Figure 1.15a. If the motion of the Lagrangian particles is tracked for a
short amount of time, the surface will look the shape in Figure 1.15b. The shaded region is unphysical and sometimes called a dovetail, fixing this problem requires complex coding procedures to find and remove the seeded points in the dovetail. A similar problem occurs if the surface fragments or undergoes a major topological change.

1.4.1.3 Two-Fluid Methods

Eulerian two-fluid methods solve multiphase flow assuming that both phases can coexist in each computational cell. Each phase has its own set of conservation equations (mass, momentum, and energy) that need to be solved. The conserved variables for each phase are weighted by the volume fraction of each fluid. This seems straightforward, but there are many terms that need to be modeled or correlated. Since many of the correlations that are needed do not exist, most of the current effort in this area has been to solve the inviscid two-fluid model which only requires one term to be modeled: the interfacial pressure between the two phases. Despite its simple appearance the inviscid two-fluid method is fraught with problems of being ill-posed [61, 62], such as loss of hyperbolicity which renders traditional shock capturing schemes ineffective. Only recently have researchers found relatively simple methods to overcome these issues and obtained some fairly impressive results on wave propagation in shocked droplets [45, 46, 58], if only for the stiffened compressible liquid equation of state.

1.4.1.4 Level Set Methods

A more complete discussion of the level set method (LSM) is given in Chapter 4. The main idea of the level set method is to capture the surface between any two arbitrary regions by moving a signed distance function, \( \phi \), that is defined to be zero at the interface. A positive signed distance function corresponds to one region and a negative signed distance function corresponds to the other. One of the distinct advantages of the LSM is that it can be used to separate domains with different physical models, with the caveat that a sufficient model for the interface must be available to couple the two domains. Because of its generality, the LSM has been used to solve a wide variety of problems including heterogeneous solid propellant combustion [63], coupling reactive gas dynamics with solid mechanics to calculate the detonation induced deformation and fracture of aluminum tubes [64], crystal growth [65], coupling a compressible gas to an incompressible liquid [66], compressible gas
and compressible liquid interactions [44, 67], low speed flames [68], and turbulent premixed flames via the so called G-equation [69]—which is really the level set equation—to name a few. Another advantage of the LSM is that calculating surface curvature and surface tension effects are accurate since the signed distance function is designed to be smooth near the interface unlike the color function used by the VOF method.

Although the LSM is very general, there is a caveat. A model of the interface between the two regions must be available to properly couple the two domains and move the interface accurately. The ghost fluid method (GFM) [67] is a popular technique for coupling two domains within a level set framework by extrapolating data from one region to another. The basic ideas of the GFM have been extended to viscous, incompressible flow with phase change [70, 71]. A relatively simple variant that works on a direction-by-direction basis was developed by Nourgaliev et al. [57, 72] for both compressible and incompressible flows.

In a detailed analysis Liu et al. [73] found some flaws with the GFM of Fedkiw et al. [67], which can transmit or reflect waves of a gas/liquid interface of the wrong type (e.g., rarefaction wave instead of a shock wave) and can have stability issues at the interface. Liu et al. [74] developed the modified ghost fluid method (MGFM) and Wang et al. [75] developed the real ghost fluid method (rGFM) which overcome the shortcomings the original GFM. Rather then fill ghost cells by extrapolating to the other, an interfacial Riemann problem is solved using an approximate Riemann solver. The solution of the Riemann problem is used to fill the ghost cells, which ensures that Riemann waves are properly transmitted and reflected at the surface. The MGFM and rGFM have been shown to be superior to the standard GFM [74, 75] and have been used to couple a compressible cavitating liquid to a gas [76].

No attempts could be found in the open literature which apply the GFM or any of its variants to compressible flows that include surface tension and/or phase change at the surface.

1.4.2 Overview of Methods for Multi-component Compressible Reacting Flow

Until recently, solving compressible multi-component reacting flows with variable specific heat ratios was a challenge. Applying standard conservative inviscid flux evaluation schemes leads to severe oscillations in pressure and velocity near a contact surface. These oscillations occur even if the pressure and velocity are initially uniform. The key to solving this problem for ideal gas mixtures with variable specific heats amounts to giving up on the notion of strict
Billet and Abgrall [77] developed a double flux model to eliminate the pressure and velocity oscillations. This technique calculates the flux at each cell edge twice, once for each cell sharing the edge. While it is not strictly conservative, the double flux model has been shown to work very well for both very low Mach number diffusion flames and flows containing shock waves [77]. The double flux model has been used to perform implicit large eddy simulation (ILES) of the interaction between a shock wave and a reacting hydrogen cylinder [77, 78] and to examine the effect of volume viscosity on the combustion processes of shocked H$_2$ bubbles [79]. The double flux model is adopted for this work and extended using modern low-dissipation methods. More details on the double flux model and low dissipation scheme are given in Chapter 3 and has been recently published in Houim and Kuo [80].

### 1.4.3 Overview of Methods for Dispersed Two-Phase Flow

Two other aspects that should be addressed are that the flow in the gas-phase region is a mixture of condensed phase alumina particles and a carrier gas. Benkiewicz and Hayashi [24] developed a numerical method capable of handling dusty compressible reacting flows. Their method assumes that the volume fraction of condensed phase particles are low enough that they can be considered “dusty”. Under the dusty assumption solids pressure is zero since the particles are assumed to be far apart. The advantage of the dusty assumption is that the wave propagation processes of the gas and dispersed phases are decoupled, avoiding the ill-posedness associated with two-fluid models and greatly simplifying the solution. This assumption, while simple, has been successfully applied to studying the interaction of shock waves with a reactive Al dust pile [24] and simulations of Al dust cloud detonations [81].

### 1.4.4 Overview of Methods for Compressible Cavitating Flows

Recently, Saurel et al. [82] developed a simple method to study supersonic cavitation over high speed projectiles. In these situations, water is not incompressible and must be treated as a compressible medium. A modified Tait liquid equation of state was used to model the compressibility of the water. Their model assumes that cavitation bubble nucleation and destruction rates are infinitely fast and that the two-phase mixture is homogeneously mixed. One downside of their work is that it is solved using a low-order MacCormack method as the base scheme to solve the Euler equations. Later, Schmidt et al. [83] extended the work of Saurel et al. [82] to a Godunov-based approach.
Liu et al. [84] developed an isentropic one-fluid model for an unsteady cavitating liquid and Xie et al. [85] developed a modified Schmidt model for barotropic cavitating liquids. Calculations of the water hammer problem using either method compare well with experimental measurements. Since they are both simple and accurate for highly transient events, both methods are adopted and combined for this work.

1.4.5 Other Modeling Considerations

Even though relative velocity between the liquid and gas can be fairly high—on the order of 1000 m/s—the Reynolds number of the droplet is not too large. Consider a very large one millimeter diameter Al droplet being accelerated by 1500 K air at 10 atm flowing at a velocity of 1000 m/s. The Reynolds number for this case would be around 40,000. The ratio of the Kolmogorov scale, η, to the prominent geometric length scale of the problem scales with $Re_d^{-3/4}$. If $\Delta x = d/f$, where $f$ is the number of computational cells per droplet diameter, we have:

$$\frac{\Delta x}{\eta} = \frac{1}{f Re_d^{-3/4}}.$$  

(1.20)

Taking $f$ to be 100, which is fairly coarse in some situations, $\Delta x/\eta = 30$. This is likely sufficient for the calculations in this work to be considered implicit large eddy simulations (ILES) [86–88] since high-order shock capturing schemes are used in this work. Favre averaged Navier-Stokes turbulence models are not appropriate since the goal of this work is to capture the unsteady dynamics of the flow field. Sub-grid large eddy simulation (LES) models for compressible multiphase chemically reacting flows could not be found. Thus, ILES is the only turbulence technique available for this work and needs to be coupled with the double-flux multi-component model and modern high-order shock capturing methods.

Another issue that is seldom brought up by the droplet combustion community is whether or not the continuum assumption is valid when the droplet size approaches the micro-scale. At very small length scales, the size of the particle becomes comparable to the mean free path, $\lambda_{mfp}$. The Knudsen number, $Kn$, is defined as the ratio of the mean free path to the relevant length scale of the computation:

$$Kn = \frac{\lambda_{mfp}}{l} = \frac{k_B T}{\sqrt{2\pi} \sigma_{coll}^2 pl}.$$  

(1.21)
where $k_B$ is the Boltzmann constant, $\sigma_{\text{coll}}$ is the molecular collision diameter. The Knudsen number determines if the flow is in the full continuum, continuum-transition, transition, or free molecular flow. The classification of flow regimes as a function of $Kn$ are given in Table 1.2. The traditional Navier-Stokes equations with no-slip boundary conditions are strictly valid in the continuum regime. When the flow regime is in the continuum-transition regime the Navier-Stokes equations can still be applied; however, partial slip boundary conditions (given in Chapter 2) should be used. In the transition regime, the Navier-Stokes equations are no longer valid, but the augmented Burnett [89] equations can be used to extend the range of validity for traditional CFD models. The augmented Burnett equations add a lengthy set of second-order terms to the viscous stresses and heat diffusion, which increases dissipation near very sharp gradients and thickens shock waves. The augmented Burnett equations really should be used if the Knudsen number approaches 0.1. Unfortunately, solving the augmented Burnett equations efficiently and stably is still a topic of research [89–91], thus the Burnett equations will not be considered in this work. Taking the representative gas temperature to be 1500 K and the collision diameter to be that of $N_2$ ($\sigma_{\text{coll}} = 3.621 \text{ Å}$), the smallest particle diameters that could be considered under the continuum approximation [based upon Eq. (1.21)] is 350 and 35 $\mu$m at atmospheric and 10 atm, respectively. The minimum particle diameter could safely be decreased to about 3.5 $\mu$m at atmospheric pressure if partial slip boundary conditions are used on the droplet surface.

### 1.5 Objectives

The main objectives of this work are listed below:

1. Develop a comprehensive model of Al droplet combustion applicable to situations involving shock waves and large slip velocities.
2. Develop a low-dissipation method for compressible reacting gas dynamic flow suitable for implicit large eddy simulation since sub-grid models are not available for complex chemically reacting multiphase flows.

3. Develop a numerical technique for coupling a compressible multi-component reacting gas to a compressible cavitating liquid with phase change and surface tension.

4. Apply the developed numerical methods to heated, vaporizing, and reacting Al droplets to obtain fundamental physical understanding of how shock waves interact with them.
As described in the introduction, a detailed model of aluminum particle combustion in a blast-wave environment requires the computation of at least three phases: a multi-component gas phase, a compressible liquid phase with cavitation, and a dispersed phase for the alumina droplets. Before the final model is discussed, general conservation equations for a multiphase reacting flow will be shown before simplifying assumptions are made and jump conditions derived at the gas/liquid interface. A discussion on the thermodynamics of ideal gas and liquid mixtures along with gaseous chemical kinetics and transport property evaluation can be found in Appendix A. Although radiation may be important, it is not considered due to its complexity and unavailability data necessary to form Plank mean absorption and scattering coefficients for many of the species involved in this thesis.

2.1 Conservation Laws

The conservation equations for mass, momentum, energy, and species mass equations can be found in many textbooks on reacting flow [5, 6, 35, 92]. Extensions to the single-phase conservations equations to compressible Eulerian multi-phase flow can be found in Ishii and Hibiki [93].
2.1.1 Conservation of Mass

The general multiphase continuity equation reads:

\[ \frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k) = \dot{m}_k''' \]  \hspace{1cm} (2.1)

where \( \alpha_k \) is the volume fraction of phase \( k \), \( \rho_k \) is the density of phase \( k \), \( \mathbf{v}_k \) is the velocity vector, and \( \dot{m}_k''' \) is a volumetric source that accounts for mass addition of phase \( k \) through evaporation, condensation, or heterogeneous chemical reactions. By definition:

\[ \sum_{i=1}^{N_{\text{phase}}} \alpha_i = 1, \]  \hspace{1cm} (2.2)

where \( N_{\text{phase}} \) is the number of phases.

2.1.2 Conservation of Momentum

The general multiphase momentum equation reads:

\[ \frac{\partial \alpha_k \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k \otimes \mathbf{v}_k) + \nabla (\alpha_k p_k) = \nabla \cdot (\alpha_k \sigma_k) + p_k,_{\text{int}} \nabla \alpha_k - \sigma_k,_{\text{int}} \nabla \alpha_k + \mathbf{v}_k,_{\text{int}} \dot{m}_k''' + \mathbf{f}_k + \mathbf{f}_k,_{\text{int}}, \]  \hspace{1cm} (2.3)

where \( \mathbf{f}_k \) accounts for other forces from within phase \( k \) such as buoyancy and \( \mathbf{f}_k,_{\text{int}} \) represents additional inter-phase forces such as drag. The tensor product \( \mathbf{v} \otimes \mathbf{v} \) is:

\[ \mathbf{v} \otimes \mathbf{v} = \begin{pmatrix} u^2 & uv & uw \\ vu & v^2 & vw \\ wu & vw & w^2 \end{pmatrix}. \]  \hspace{1cm} (2.4)

The term \( p_k,_{\text{int}} \nabla \alpha_k \) is analogous to the \( p \, dA \) term in variable area duct flow and is sometimes called a “nozzling term” [94] and represents the force acting on a phase due to gradients in the volume fraction. The net stress acting on the interface of phase \( k \) is \( \sigma_{k,\text{int}} \cdot \nabla \alpha_{k,\text{int}} \). The interfacial terms \( p_{k,\text{int}}, \sigma_{k,\text{int}}, \) and \( \mathbf{v}_{k,\text{int}} \) need to be modeled or correlated.

The deviatoric stress tensor, \( \sigma \), is defined by:

\[ \sigma_{xx,k} = 2\mu_k \frac{\partial u_k}{\partial x} + (\kappa - \frac{2}{3} \mu) \nabla \cdot \mathbf{v}_k, \]  \hspace{1cm} (2.5)
\[
\sigma_{yy,k} = 2\mu_k \frac{\partial v_k}{\partial y} + (\kappa - \frac{2}{3}\mu)\nabla \cdot \mathbf{v}_k, \tag{2.6}
\]
\[
\sigma_{xy,k} = \sigma_{yx,k} = \mu_k \left( \frac{\partial u_k}{\partial y} + \frac{\partial v_k}{\partial x} \right), \tag{2.7}
\]

where \(\mu_k\) is the shear viscosity and \(\kappa_k\) is the bulk (or volume) viscosity.

The divergence of velocity is:
\[
\nabla \cdot \mathbf{v}_k = \frac{\partial u_k}{\partial x} + \frac{1}{y^\eta} \frac{\partial y^\eta v_k}{\partial y}, \tag{2.8}
\]
where \(\eta\) is a parameter that selects between 2-D Cartesian, 2-D axisymmetric, or 1-D spherical (\(\eta = 2\)):
\[
\eta = \begin{cases} 
0 & \text{cartesian} \\
1 & \text{axisymmetric} \\
2 & \text{spherical (1-D)}. 
\end{cases} \tag{2.9}
\]

### 2.1.3 Conservation of Species Mass

The general conservation equation of mass for species \(i\) in phase \(k\) is:
\[
\frac{\partial \alpha_k \rho_k Y_{k,i}}{\partial t} + \nabla \cdot (\alpha_k \rho_k Y_{k,i} \mathbf{v}_k) + \nabla \cdot (\alpha_k \mathbf{J}'_{k,i}) = \dot{\omega}'_{k,i} + \dot{\omega}'_{k,i,H}, \tag{2.10}
\]
where \(Y_{k,i}\) is the mass fraction of species \(i\) in phase \(k\), \(\mathbf{J}'_{k,i}\) is the diffusion flux of species \(i\) in phase \(k\), and \(\dot{\omega}'_{k,i}\) and \(\dot{\omega}'_{k,i,H}\) represent the mass production rate of species \(i\) by homogeneous and heterogeneous chemical reactions, respectively. Conservation of mass dictates that \(\sum_i \dot{\omega}'_{k,i} = 0\) and \(\sum_k \dot{\omega}'_{k,i,H} = \dot{m}'_{k}\).

The mass diffusion flux is defined as:
\[
\mathbf{J}'_{k,i} = \rho_{k,i} Y_{k,i} \mathbf{V}_{k,i}, \tag{2.11}
\]
where \(\mathbf{V}_{k,i}\) is the diffusion velocity of species \(i\) in phase \(k\). To decrease computational expense, a simplified mixture-averaged formulation [35] is used to evaluate diffusion velocity:
\[
\bar{\mathbf{V}}_{k,i} = -\frac{D_{k,i,\text{mix}}}{X_{k,i}} \mathbf{D}_{k,i} - \frac{D_{T,k,i}}{\rho_{k,i} Y_{k,i}} \nabla (\ln T), \tag{2.12}
\]
where the potential for mass diffusion, $D_{k,i}$, is:

$$D_{k,i} = \nabla X_{k,i} + (X_{k,i} - Y_{k,i}) \nabla (\ln p)$$  \hspace{1cm} (2.13)

and $D_{k,i,mix}$ is the mixture-averaged diffusion coefficient. The first term in the diffusion velocity is analogous to Fickian diffusion, the second term is pressure diffusion (sometimes called barodiffusion), and the last term represents the Soret effect which is mass diffusion due to temperature gradients. The Soret effect is only important in situations with large temperature gradients such as premixed flames and only if very light species such as H, He, H$_2$, etc. are present in the gaseous mixture. Since all of the species considered in this model are relatively heavy, the Soret effect is neglected.

One problem using mixture-averaged mass diffusion is that mass is not necessarily conserved (i.e., $\sum J''_i \neq 0$). To circumvent this, the correction velocity, $V_{k,c}$, of Coffee and Hiemerl [35, 95] is used:

$$V_{k,c} = - \sum_{i=1}^{N_g} Y_{k,i} \tilde{V}_{k,i} k_i$$  \hspace{1cm} (2.14)

where $N_g$ is the number of species in the gas phase and $\tilde{V}_{k,i}$ is the diffusion velocity evaluated from Eq. (2.12). The diffusion velocity used to evaluate the diffusion flux is:

$$V_{k,i} = \tilde{V}_{k,i} + V_{k,c}.$$  \hspace{1cm} (2.15)

Note that all of the species equations and the continuity equation are not linearly independent, since conservation of mass demands that summing all species mass equations produces the continuity equation. Two popular options are to solve $N_g - 1$ species equations and the continuity equation and use the definition of mass fraction to obtain the mass fraction of chemical species $N_g$. Another approach (and the one used in this work) is to simply solve all $N_g$ species equations without the continuity equation, which implicitly satisfies continuity.
2.1.4 Conservation of Energy

A generic energy equation for a compressible multiphase flow is:

\[
\frac{\partial \alpha_k \rho_k E_k}{\partial t} + \nabla \cdot (\alpha_k \mathbf{v}_k (\rho_k E_k + p_k)) = -\nabla \cdot (\alpha_k \mathbf{q}_k) + \nabla \cdot (\sigma_k \cdot \mathbf{v}_k) - p_k \frac{\partial \alpha_k}{\partial t} \\
+ \dot{m}^{m}_k \left( h_{k,\text{int}} + \mathbf{v}_{k,\text{int}} \cdot \mathbf{v}_k - \frac{\mathbf{v}_k \cdot \mathbf{v}_k}{2} \right) + a_{\text{int}} \dot{q}_{k,\text{int}}'' - \left( \nabla \alpha_k \cdot \sigma_{k,\text{int}} \right) \cdot \mathbf{v}_{k,\text{int}} \\
+ \mathbf{f}_k \cdot \mathbf{v}_k + \mathbf{f}_{k,\text{int}} \cdot \mathbf{v}_{k,\text{int}} + \dot{Q}'''' + \dot{W}''''_{k,\text{int}},
\]

where \( E_k \) is the specific total internal energy (\( E = e + \mathbf{v} \cdot \mathbf{v} / 2 \)), \( \mathbf{q} \) is the diffusion heat flux vector, and \( \dot{Q}'''' \) is a source term that can account for volumetric energy sources such as radiation. Note that the internal energy, \( e \), includes both sensible and chemical energy. The term \( p_k \frac{\partial \alpha_k}{\partial t} \) represents the work loss from phase \( k \) due the time-rate-increase in volume fraction and is is sometimes written as a “nozzling term”, \( p_k \mathbf{v}_k \cdot \nabla \alpha_k \) [94]. At first glance this term may seem a little strange; however, it physically represents the work transferring from one phase to another due to a change in volume fraction. In addition to the work done by the moving interface and energy associated with phase change, there may be additional heat \( a_{\text{int}} \dot{q}_{k,\text{int}}'' \) and work generated at the interface \( \dot{W}''''_{k,\text{int}} \). Since the definition of internal energy and enthalpy includes chemical energy, there is no need to explicitly model energy source terms from homogeneous chemical reactions.

The diffusion heat flux vector is:

\[
\mathbf{q} = \sum_{i=1}^{N_g} J''_{k,i} h_{k,i} \mathbf{v}_k - \lambda_k \nabla T_k - \sum_{i=1}^{N_g} \frac{R_u T D'_{i} T_{D} F_{i}}{Mw_i X_{i}} D_{k,i}, \tag{2.17}
\]

where \( R_u \) is the universal gas constant and \( Mw_i \) is the molecular weight of species \( i \). The first term represents heat transported by mass diffusion, the second term is Fourier’s Law where \( \lambda_k \) is the mixture thermal conductivity of phase \( k \). The last term is the Dufour effect which is a second order effect that is usually smaller than the Soret effect, thus it is neglected.

2.1.5 Model Simplifications

As mentioned in the introduction, applying the above multiphase equations is very difficult and requires the use of many approximations and correlations to estimate terms such as interphase stress. Since the overall goal of this work is to calculate the detailed combustion
2.1 Figure 2.1: Sketch of gas and liquid regions considered in this model.

processes of a single Al droplet interacting with a shock wave, the multiphase equations can be greatly simplified by “zooming” in on a single droplet and separating the domain into two regions as shown in Figure 2.1.

The entire domain was split into two separate sub-domains; a gas-phase region and a liquid-phase region separated by an infinitesimal interface. Each region has its own set of governing equations that are coupled at the interface through jump conditions. Note that the aluminum oxide layer and lobe are neglected due to the destruction of the original alumina shell during the detonation process of the high-explosive charge [15, 16]. Ignition is not considered since this thesis is focused on burning Al droplets that outrace the contact surface of the high-explosive charge, burn in air, and interact with reflected shock waves. As stated in Chapter 1, dissolution of gas-phase species into liquid aluminum is not taken into account.

2.2 Model for the Gas-Phase Region

In the gas-phase region, there are two distinct phases; the gas phase and condensed phase alumina droplets. Since the condensed phase alumina droplets are nano-sized and have a relatively small volume fraction when Al droplets burn with air, they can be treated in the dusty limit [24]. In this limit heat conduction, terms analogous to viscous stresses in the
condensed phase, and solids pressure can be neglected since each dust particle is essentially isolated from other dust particles. Using the dusty assumption and neglecting buoyancy, the governing equations for the gas-phase in the gaseous region reduce to [24]:

\[
\frac{\partial \rho_g Y_{g,i}}{\partial t} + \nabla \cdot (\rho_g Y_{g,i} \mathbf{v}_g) + \nabla \cdot \mathbf{J}_{g,i}'' = \dot{\omega}_{g,i}'' - \frac{\dot{\omega}_{g,i}'' \rho_g}{1 - \alpha_c}, \quad (2.18)
\]

\[
\frac{\partial \rho_g \mathbf{v}_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{v}_g \otimes \mathbf{v}_g) + \nabla p - \nabla \cdot \mathbf{\sigma}_g = \frac{(\dot{m}_g'' - F_d)(\mathbf{v}_g - \mathbf{v}_c) + \dot{h}_{g''} (E_c - E_g)^{\alpha_c}}{1 - \alpha_c} - \mathbf{F}_T, \quad (2.19)
\]

and

\[
\frac{\partial \rho_g E_g}{\partial t} + \nabla \cdot (\rho_g E_g \mathbf{v}_g) - \nabla \cdot (\sigma_g \cdot \mathbf{v}_g) = \dot{m}_g'' (E_c - E_g)_{\alpha_c} + \dot{h}_{g''} (T_g - T_c) + \mathbf{F}_T \cdot \mathbf{v}_c, \quad (2.20)
\]

where \( h \) is the heat transfer coefficient between the condensed phase particles and the gas phase, \( F_d \) is the interphase drag force factor, \( \mathbf{F}_T \) is the thermophoresis force, \( N_c \) is the number density of the condensed particles, and \( \alpha_c \) is the volume fraction of the condensed phase. The ideal gas law is assumed for the gaseous equation of state.

The condensed phase equations are quite similar, with the exception that solids pressure does not affect particle momentum due to the dusty assumption and a scalar equation for the particle number density, \( N_c \), is added:

\[
\frac{\partial \alpha_c \rho_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c \mathbf{v}_c) = -\dot{m}_g'', \quad (2.21)
\]

\[
\frac{\partial \alpha_c \rho_c \mathbf{v}_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c \mathbf{v}_c \otimes \mathbf{v}_c) = -\dot{m}_g'' \mathbf{v}_g - \dot{h}_{g''} \mathbf{v}_c - \dot{m}_g'' \mathbf{v}_c + \mathbf{F}_T, \quad (2.22)
\]

\[
\frac{\partial \alpha_c \rho_c E_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c E_c \mathbf{v}_c) = -\dot{m}_g'' \mathbf{v}_g - \dot{h}_{g''} (E_c - E_g)_{\alpha_c} + \mathbf{F}_T \cdot \mathbf{v}_c, \quad (2.23)
\]

and

\[
\frac{\partial N_c}{\partial t} + \nabla \cdot (N_c \mathbf{v}_c) = J_c, \quad (2.24)
\]

where \( J_c \) is a source term for the condensed phase number density. While the assumption of negligible alumina volume may not be perfect at all times, it decouples the hyperbolic and parabolic terms of the two phases. This decoupling removes the host of problems that plague
Table 2.1: Gaseous Al/O reaction mechanism [11]; $k_f = AT^n \exp(-E_a/R_uT)$.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>$A$ (mol/cm$^3$ s)</th>
<th>$n$</th>
<th>$E_a$(cal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Al + O$_2$ ⇌ AlO + O</td>
<td>$9.72 \times 10^{13}$</td>
<td>0.0</td>
<td>159.95</td>
</tr>
<tr>
<td>2</td>
<td>Al + O + M ⇌ AlO + M</td>
<td>$3.00 \times 10^{17}$</td>
<td>-1.0</td>
<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>AlO + O$_2$ ⇌ AlO$_2$ + O</td>
<td>$4.62 \times 10^{14}$</td>
<td>0.0</td>
<td>19885.90</td>
</tr>
<tr>
<td>4</td>
<td>Al$_2$O$_3$ ⇌ Al$_2$O$_2$ + O</td>
<td>$3.00 \times 10^{15}$</td>
<td>0.0</td>
<td>97649.99</td>
</tr>
<tr>
<td>5</td>
<td>Al$_2$O$_3$ ⇌ AlO$_2$ + AlO</td>
<td>$3.00 \times 10^{15}$</td>
<td>0.0</td>
<td>126999.89</td>
</tr>
<tr>
<td>6</td>
<td>Al$_2$O$_2$ ⇌ AlO + AlO</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>117900.00</td>
</tr>
<tr>
<td>7</td>
<td>Al$_2$O$_2$ ⇌ Al + AlO$_2$</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>148900.00</td>
</tr>
<tr>
<td>8</td>
<td>Al$_2$O$_2$ ⇌ Al$_2$O + O</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>104249.94</td>
</tr>
<tr>
<td>9</td>
<td>AlO$_2$ ⇌ AlO + O</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>88549.86</td>
</tr>
<tr>
<td>10</td>
<td>Al$_2$O ⇌ AlO + Al</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>133199.94</td>
</tr>
</tbody>
</table>

other two-fluid methods such as loss of hyperbolicity [61], and allows the use of solvers that work best for each phase independently.

Assuming that the condensed phase alumina particles have a uniform size distribution in each computational cell, the particle volume averaged diameter can be calculated from the volume fraction via:

$$r_c = \frac{1}{2} \left( \frac{6 \alpha_c}{\pi N_c} \right)^{1/3}.$$  

(2.25)

2.2.1 Gas-Phase Chemical Reactions

The calculation procedure for the chemical reaction source term $\dot{\omega}^{'''}_{g,i}$ is discussed in Appendix A. Even though there are many instances when an Al droplet may react with water vapor and carbon dioxide in propulsion and explosive applications, this work is primarily focused on shock waves interacting with Al droplets in air. The chemical mechanism adopted for this work is that of Huang et al. [11] and is given in Table 2.1.

Detailed reaction mechanisms involving gaseous Al with hydrogen, oxygen, chlorine, and carbon have been developed [23, 96, 97]; however, there are too many species and chemical reactions in these mechanisms to be practical for the detailed calculations in this work. If any of these more complete mechanisms are considered in future work, a significant effort should be spent reducing these mechanisms to a manageable size.
2.2.2 Particle Drag and Thermophoresis

The interphase drag factor is calculated by summing the drag force acting on all particles within the control volume. Treating each particle as a sphere the total drag force on all particles in the control volume, \( F_d \), is:

\[
F_d = \frac{\pi}{8} d^2 c N c \rho g |v_g - v_c| (v_g - v_c), \tag{2.26}
\]

then

\[
F_d = \frac{3}{2} \alpha_c C_d \rho g |v_g - v_c|. \tag{2.27}
\]

Although complex expressions exist for estimating the drag coefficient for particles in subsonic and supersonic flows such as Henderson [98], a simplified drag correlation is used due to its ease of numerical implementation. Benkiewicz et al. [24] point out that when the particles are small, the velocity of the particles and the gas equilibrate rapidly and the form of the drag coefficient used has a relatively small effect on computed results. The drag coefficient is calculated using the correlation of Carlson and Hoglund [99]:

\[
C_d = \frac{24}{R ed} \left[ \frac{(1 + 0.15 Re d^{0.687})(1 + \exp[0.427/M^{4.63} - 3/Re d^{0.88}])}{1 + \frac{M}{Re d}(3.82 + 1.28 \exp[-1.25 Re d/M])} \right], \tag{2.28}
\]

where \( M \) is the Mach number of the particle based on the relative velocity between the gas and particles and \( Re d \) is the Reynolds number of the particles based on the diameter and relative velocity between the particles and the gas. It can be shown from kinetic theory that \( Kn = M/Re \sqrt{\gamma \pi/2} \), thus the terms in Eq. (2.28) involving \( M/Re d \) represent a correction for high Knudsen number particles. Equation (2.28) does not include the effects of phase change on particle drag. Correlations for drag that account for the influence of phase change can be found in Yarin and Hetsroni [100].

Another force that becomes important for small particles in flows that involve sharp temperature gradients is thermophoresis, \( F_T \). Thermophoresis is a force that acts on particles due to temperature gradients in the gas carrying them and is analogous to the Soret effect. Thermophoresis is calculated using equation developed by Talbot [101]:

\[
F_T = -\frac{12 \pi r_c N c \mu g^2 C_s (K + 2 C_t Kn)}{\rho g (1 + 6 C_m Kn)(1 + 2K + 4C_t Kn)} \nabla (\ln T), \tag{2.29}
\]
where $Kn$ is the Knudsen number of the particles (recall that $Kn \equiv \lambda_{mfp}/d_c$), $C_s = 1.17$, $C_t = 2.18$, $C_m = 1.14$, and

$$K \equiv \frac{15}{4} \frac{\mu_g R_u}{Mw_g \lambda_c}.$$  \hspace{1cm} (2.30)

### 2.2.3 Heat Transfer to Alumina Droplets

The overall heat transfer coefficient between the particles and the gas is:

$$h = \frac{6\alpha_cNu_d\lambda_g}{d_c^2},$$  \hspace{1cm} (2.31)

where $Nu$ is the Nusselt number of a single particle given by the correlation of Carlson and Hoglund [99]:

$$Nu_d = \frac{2 + 0.459 Re_c^{0.55} Pr_g^{0.33}}{1 + 3.42 \frac{M}{Re_c Pr_g} (2 + 0.459 Re_c^{0.55} Pr_g^{0.33})},$$  \hspace{1cm} (2.32)

where the Mach and Reynolds numbers are based on the relative velocity between the gas and the particles. Viscosity and thermal conductivity are evaluated at the local gas temperature rather than the film temperature to reduce the number of expensive transport property evaluations. The denominator of Eq. (2.32) represents a correction for high Knudsen number particles.

### 2.2.4 Alumina Condensation

The formation and subsequent condensation of a liquid droplet consists of two distinct phases; nucleation and condensation. Internally consistent homogeneous nucleation theory [102] is used to calculate the nucleation rate:

$$J_c = \sqrt{\frac{2\sigma_t}{\pi m_1 v_1 S}} \left( \frac{p_{\text{sat}}}{k_BT} \right)^2 \exp \left[ -\frac{16\pi}{3} \frac{v_1^2 \sigma_t^3}{k_B T^3 (\ln S)^2} + \frac{\sigma_t A_0}{k_BT} \right],$$  \hspace{1cm} (2.33)

where $S$ is the supersaturation ratio $S \equiv p_{\text{vap}}/p_{\text{sat}}$, $\sigma_t$ is the surface tension, and $N_1$, $m_1$, and $v_1$ are the number, mass, and volume of a monomer (i.e., one “liquid” molecule) respectively, and $A_0 = (36\pi v_1^2)^{1/3}$. The size of the condensed phase nuclei, the critical radius $r^*$ must also be known to determine the mass exchange between the gas and liquid phases. Using the Kelvin equation:

$$r^* = \frac{2\sigma_t v_1}{k_BT \ln S}.$$  \hspace{1cm} (2.34)
Mass exchange between the gas and condensed phases due to nucleation is:

\[
\dot{m}''_{g,nuc} = -\frac{4}{3}\pi \rho_{Al_2O_3(l)} r^3 J_c. \tag{2.35}
\]

After particles have been nucleated, they continue to grow due to condensation; coagulation of alumina droplets is not considered in this model. The coagulation mechanisms presented in Chapter 13 of Seinfeld and Pandis [9] could be adopted to consider particle coagulation in future studies. The condensation rate is simply [9]:

\[
\dot{m}''_{g,cond} = -\frac{4\pi N_c r_c \mathcal{D}_{Al_2O_3,mix} M_{w,Al_2O_3}}{R_u T} \frac{1 + Kn_c}{1 + 2Kn_c(1 + Kn_c)}(p_{Al_2O_3} - p_{sat,Al_2O_3}), \tag{2.36}
\]

where \( \mathcal{D}_{Al_2O_3,mix} \) is the mixture-averaged “gaseous” alumina diffusion coefficient, \( r_c \) is the radius of the droplets in a given volume, and \( Kn_c \) is the Knudsen number with the mean free path defined as:

\[
\lambda_{mfp} = 2\mathcal{D}_{Al_2O_3,mix} \sqrt{\frac{\pi M_{w,Al_2O_3}}{8R_u T}}. \tag{2.37}
\]

In Eq. (2.36), the multiplier accounting for high Knudsen number effects is called the Dahneke correction. Without the Dahneke correction, the condensation rate of small droplets follows the continuum approximation and would be overestimated.

For most fluids the saturation pressure is known as a function of temperature; however, alumina dissociates before it vaporizes. Thus, the concept of alumina saturation pressure and even gaseous alumina is not physical. However, “gaseous” alumina is used for computational convenience and other means are explored to obtain a saturation pressure because empirical measurements are out of the question. Ideally, the alumina condensation mechanism based on homogeneous nucleation theory developed by Beckstead et al. [22] could be utilized; however, this method requires the use of empirically determined model parameters that were tuned so that the model results produced good agreement with experimental aluminum particle burning times. Unfortunately the authors never mentioned the tunable parameters that worked for them, rendering their novel alumina condensation mechanism essentially useless to other researchers.

Another approach used by Huang et al. [11] treats the condensed-phase alumina droplets as a separate gas-phase component in addition to gaseous alumina. The condensation reaction is treated as a reversible unimolecular homogeneous gas-phase reaction with zero activation energy and a high pre-exponential factor. In addition to its simplicity the flame
temperature of aluminum, which is determined largely by the dissociation temperature of alumina [20], is computed naturally from equilibrium thermodynamics rather than using ad-hoc functions that force alumina dissociation if the temperature is too high [22, 24]. While the entirely gas-phase (or homogeneous) method was designed to compute the combustion of aluminum particles approaching the molecular limit, is it not completely appropriate for larger particles where the dynamics of the condensed phase alumina may play an important role.

In this work the unimolecular reaction approach was used to define an effective alumina saturation pressure. This effective saturation pressure will be used to evaluate the nucleation and condensation rates. Examining the condensation reaction of [11]:

$$\text{Al}_2\text{O}_3 \xrightleftharpoons[k_f]{k_r} \text{Al}_2\text{O}_3(l)$$  \hspace{1cm} (2.38)

and applying the partial equilibrium assumption:

$$k_f[\text{Al}_2\text{O}_3] = k_r[\text{Al}_2\text{O}_3(l)] = k_r([\text{Al}_2\text{O}_3(tot)] - [\text{Al}_2\text{O}_3]),$$  \hspace{1cm} (2.39)

we find that

$$p_{\text{Al}_2\text{O}_3,\text{sat}} = \frac{R_u T}{M_{\text{Al}_2\text{O}_3}} \frac{1}{K_c + 1} [(1 - \alpha_c)\rho_3 Y_{\text{Al}_2\text{O}_3} + \alpha_c \rho_{\text{Al}_2\text{O}_3(l)}],$$  \hspace{1cm} (2.40)

where $[\text{Al}_2\text{O}_3(tot)]$ is the total alumina concentration (both “gaseous” and dispersed phase) and $K_c$ is the equilibrium constant. Using the alumina saturation pressure defined by Eq. (2.40) allows the use of homogeneous nucleation theory without the need for tunable parameters. When the alumina saturation pressure is zero, the condensation rate of alumina is taken to be zero.

### 2.3 Model for the Liquid Region

Similar to the gas-phase region, there exists two different phases in the liquid region: liquid and a dispersed bubbly phase. The bubbly phase corresponds to vapor that may have formed due to cavitation in the droplet. A similar approach to the condensed phase alumina could be used for the vapor bubbles; however, the volume of the vapor bubbles is not negligible. Also, drag forces restoring mechanical equilibrium between bubbles and the liquid are much
greater than they are between gas and particles. Thus, it is assumed that the bubbles and the liquid are homogeneously mixed, requiring the solution of one momentum and energy equation. Furthermore, a barotropic equation of state suitable for a compressible, cavitating liquid is assumed.

As stated in the introduction, during the combustion of aluminum particles an aluminum oxide cap usually forms on the droplet. Since liquid Al and alumina are technically immiscible, they should be treated as two separate liquid phases for a physically correct approach. Current interface tracking methodology for computational physics have only treated one interface (or two sub-domains). Although multiple sub-domains have been computed using multiple level set equations for the computer graphics industry [103], adding another sub-domain to computational physics calculations is a research topic itself. To simulate any layer of liquid alumina that may form at the droplet surface, the liquid phase is treated as a mixture of liquid alumina and liquid aluminum, with mass diffusion between liquid aluminum and liquid alumina neglected to imitate immiscibility. The only mixing of aluminum and alumina occurs due to numerical dissipation. Absorption of gas-phase species is not considered. As with the gas-phase region, a detailed discussion on liquid equations of state and mixing rules can be found in Appendix A.

Using the above assumptions, the governing equations for the liquid region are:

\[
\frac{\partial \alpha_l \rho_l Y_{Al}}{\partial t} + \nabla \cdot (\alpha_l \rho_l Y_{Al} \mathbf{v}) = -\dot{S}_{cav},
\]

\[
\frac{\partial \alpha_l \rho_l Y_{Al_2O_3}}{\partial t} + \nabla \cdot (\alpha_l \rho_l Y_{Al_2O_3} \mathbf{v}) = 0,
\]

\[
\frac{\partial (1 - \alpha_l) \rho_v}{\partial t} + \nabla \cdot ((1 - \alpha_l) \rho_v \mathbf{v}) = \dot{S}_{cav},
\]

\[
\frac{\partial \rho_m \mathbf{v}}{\partial t} + \nabla \cdot (\rho_m \mathbf{v} \otimes \mathbf{v}) = -\mathbf{\nabla} p + \mathbf{\nabla} \cdot \mathbf{\sigma},
\]

\[
\frac{\partial \rho_m E_m}{\partial t} + \nabla \cdot (\rho_m E_m + \mathbf{p}) = -\mathbf{\nabla} \cdot \mathbf{q} + \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{v}),
\]

where \( \alpha_l \) is the liquid volume fraction. The mixture density \( \rho_m \) and energy \( E_m \) are mixed based on the volume fraction:

\[
\rho_m = \alpha_l \rho_l + (1 - \alpha_l) \rho_v.
\]
The thermal conductivity and viscosities (both shear and bulk) are mixed based on the volume fraction as well. Tait’s equation of state is used for the liquid and the isentropic equation of state is used for the bubbles (see Appendix A). The saturation pressure of the liquid aluminum in the mixture is calculated using Raoult’s law. Raoult’s law states that saturation pressure of liquid component $i$ in a mixture is given by:

$$p_{\text{sat,mix},i} = X_i p_{\text{sat,pure},i},$$  \hspace{1cm} (2.47)

where $X_i$ is the mole fraction of species $i$ in the liquid mixture.

The mixture speed of sound between the bubbly and the continuous phase is calculated using the results of Wallis [104]:

$$\frac{1}{\rho_m c_m^2} = \frac{\alpha_l}{\rho_l c_l^2} + \frac{1 - \alpha_l}{\rho_v c_v^2},$$  \hspace{1cm} (2.48)

where $c_l$ and $c_v$ are the speeds of sound in pure liquid and pure vapor, respectively. It is interesting to note that two-phase mixtures have a sound speed that is far lower than the sound speed for each pure component. The mixture sound speed for mixtures of liquid and vapor Al at 933 K as a function of liquid volume fraction is shown in Figure 2.2. A more detailed discussion of the two-phase speed of sound can be found in [105].

**Figure 2.2:** Sound speed of liquid/vapor Al mixtures at 933 K.
There are several methods to model the cavitation of a compressible liquid. Saurel et al. [82] and Schmidt et al. [83] assume that vapor and liquid are in thermodynamic equilibrium and that vapor bubbles nucleate and collapse infinitely fast. Liu et al. [84] developed an isentropic one-fluid model of cavitation. More traditional finite rate cavitation models such as Singhal et al. [106] or Bakir et al. [107] are not designed for rapid depressurization events and may not be suitable for this work. Since they work well with the level set method and rapid depressurization events, the one-fluid isentropic model of Liu et al. [84] and the modified Schmidt model of Xie et al. [85] are adopted and combined. This model does not calculate the cavitation rate explicitly and does not have the need to separate the mass conservation equations for each phase, which simplifies the governing equations for the liquid region to:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0, \\
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) &= -\nabla p + \nabla \cdot \sigma, \\
\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{v}) &= -\nabla \cdot \mathbf{q},
\end{align*}
\]

where \( e = e_{\text{ref}} + C_v(T - T_{\text{ref}}) \). For a liquid, \( h = e + pv \approx e \) since the specific volume is very low at moderate pressures. The key to using one-fluid barotropic cavitation models is to determine an accurate equation of state that is numerically simple to implement. The equation of state is split into three regions: pure liquid \((p \geq p_{\text{sat}})\), moderately cavitating liquid \((p_{\text{cav}} < p < p_{\text{sat}})\), and strongly cavitating liquid \((p \leq p_{\text{cav}})\). The cavitation pressure, \( p_{\text{cav}} \), is related to the saturation pressure, \( p_{\text{sat}} \), by \( p_{\text{cav}} = \chi_{\text{cav}} p_{\text{sat}} \), where \( 0 < \chi_{\text{cav}} < 1 \).

If the pressure of the liquid is greater than the saturation pressure, \( p_{\text{sat}} \), or the density is greater than the density at the saturation pressure, the fluid is a pure liquid and the Tait equation of state is employed:

\[
p_{\text{Tait}} = B \left[ \left( \frac{\rho}{\rho_{\text{ref}}} \right)^N - 1 \right] + A,
\]

where \( A, B, N, \) and \( \rho_{\text{ref}} \) are physical constants. The speed of sound for a Tait liquid is given by:

\[
c_{\text{Tait}} = \sqrt{\frac{N(p + B - A)}{\rho}}.
\]
In the moderately cavitating region \((p_{\text{cav}} < p < p_{\text{sat}})\) the modified Schmidt (m-Schmidt) model \([85]\) is used. The pressure for the m-Schmidt model is:

\[
p_{\text{m-Schmidt}} = p_{\text{sat}} + p_{gl} \ln \left[ \frac{\rho_{gs} c_{gs}^2 (\rho_{ls} + \alpha (\rho_{gs} - \rho_{ls}))}{\rho_{ls} (\rho_{gs} c_{gs}^2 - \alpha (\rho_{gs} c_{gs}^2 - \rho_{ls} c_{ls}^2))} \right],
\]

where \(\alpha\) is the vapor volume fraction, \(\rho_{gs}\) and \(\rho_{ls}\) are the densities of the vapor and liquid phase at the saturation pressure, \(c_{gs}\) and \(c_{ls}\) are the sound speeds of the vapor and liquid phases at the saturation pressure, and

\[
p_{gl} = \frac{\rho_{gs} c_{gs}^2 \rho_{ls} c_{ls}^2 (\rho_{gs} - \rho_{ls})}{\rho_{gs} c_{gs}^2 - \rho_{ls} c_{ls}^2}.
\]

The volume fraction of the vapor phase is determined from its definition via \(\alpha_{\text{m-Schmidt}} = \frac{(\rho - \rho_{ls})}{(\rho_{gs} - \rho_{ls})}\). The sound speed for the m-Schmidt model is:

\[
c_{\text{m-Schmidt}} = \left\{ \rho \left[ \frac{\alpha}{\rho_{gs} c_{gs}^2} + \frac{1 - \alpha}{\rho_{ls} c_{ls}^2} \right] \right\}^{-1/2}.
\]

In the strongly cavitating region \((p \leq p_{\text{cav}})\) the isentropic one-fluid (m-Isen) model \([84]\) is utilized, which has been slightly modified for this work. Using the isentropic one-fluid model, the pressure is calculated implicitly from density:

\[
\rho_{\text{m-Isen}} = C \frac{k_{\text{cav}} \rho_{gc} + \rho_{lc}}{\left( \frac{p + B - A}{p_{\text{cav}} + B - A} \right)^{-1/\gamma} + k_{\text{cav}} \left( \frac{p}{p_{\text{cav}}} \right)^{-1/\gamma}}
\]

where \(\rho_{gc}\) and \(\rho_{lc}\) are the densities of the vapor and liquid phases at the cavitation pressure, \(\gamma\) is the specific heat ratio of the vapor,

\[
k_{\text{cav}} = \frac{\alpha_{\text{m-Schmidt}} (p_{\text{cav}})}{1 - \alpha_{\text{m-Schmidt}} (p_{\text{cav}})};
\]

and

\[
C = \frac{\rho_{\text{m-Schmidt}} (p_{\text{cav}})}{\alpha_{\text{m-Schmidt}} (p_{\text{cav}}) \rho_{gc} + [1 - \alpha_{\text{m-Schmidt}} (p_{\text{cav}})] \rho_{lc}}.
\]

When solving the conservation equations for the liquid phase, density is known and the pressure needs to be calculated. Pressure is solved from Eq. (2.57) using Newton’s
method. Typically only five or less iterations are needed to achieve an error less than or equal to $10^{-14}$. Once pressure is known, the volume fraction can calculated directly by

$$\alpha_{m-Iesen} = \frac{\rho - \rho_l(p)}{\rho_g(p) - \rho_l(p)}.$$ 

Finally, the speed of sound for the modified isentropic one-fluid model is:

$$c_{m-Iesen} = \left\{ \rho \left[ \frac{\alpha}{\gamma p} + \frac{1 - \alpha}{N(p + B - A)} \right] \right\}^{-1/2}. \quad (2.60)$$

A plot of the density and sound speed for water ($\rho_{ref} = 1000 \text{ kg/m}^3$, $A = 10^5 \text{ Pa}$, $B = 3.31 \times 10^8 \text{ Pa}$, $N = 7.15$, $p_{sat} = 2 \text{ kPa}$, and $\chi_{cav} = 0.9$) is shown in Figure 2.3. Note that this equation of state is strictly convex (i.e., the flux vector increases with increasing conserved variables) and an exact solution to the Riemann problem can be constructed. If the equation of state is not convex then additional complications resulting from expansion shocks and compression fans need to be considered [108–110]. Since the liquid phase region does not contain material interfaces (barotropic equations of state do not contain contact surfaces) and the time scales for the calculations in this work are quite short (less than five microseconds), the droplet temperature does not change very much and the parameters for liquid equation of state are chosen to be constant.
2.4 Coupling the Gas and Liquid Regions

Now that the governing equations for each region have been developed, a method for coupling them at the interface must be derived for mass, momentum, energy, and species conservation. In this section it is understood that $u_n$ corresponds to the velocity normal to the surface, $u_t$ is the velocity tangential to the interface, $\sigma_{nn}$ is the deviatoric stress in the normal direction at the interface, and $\sigma_{nt}$ is the shear stress at the interface. If a generic control volume in Figure 2.4 is considered and a general flux balance of a scalar $b$ is performed, the Reynolds transport theorem at an interface is derived. Since we are interested in quantities across the interface, only the thickness of the control volume will tend to zero. Any flux entering the control volume tangentially is not considered due to the small face area on the sides in comparison to the top and bottom faces. Also, any volumetric quantity will tend to zero since the volume scales with $\epsilon$. Assuming that the control volume moves at velocity $v_b$, the Reynolds transport theorem,

$$\frac{DB_{sys}}{Dt} = \iint_{CV} \frac{\partial \rho b}{\partial t} dV + \iint_{CS} \rho b (v - v_I) \cdot \hat{n} dA,$$

is reduced to:

$$\frac{DB_{sys}}{Dt} = [\rho_g b_g (u_{n,g} - u_{n,I}) - \rho_l b_l (u_{n,l} - u_{n,I})] A.$$
at an interface where \( u_n = \mathbf{v} \cdot \hat{n} \) and \( u_{n,I} = \mathbf{v}_I \cdot \hat{n} \). Similarly, only surface effects (with the exception of surface tension) on top and bottom faces of the control volume need to be considered.

### 2.4.1 Interfacial Mass Balance

Consider the control volume shown in Figure 2.5. Performing an overall mass balance for a control volume that moves with the surface at velocity, \( \mathbf{v}_I \) gives:

\[
\alpha_c \rho_c (u_{n,c} - u_{n,I}) + \alpha_g \rho_g (u_{n,g} - u_{n,I}) = \alpha_l \rho_l (u_{n,l} - u_{n,I}) + \alpha_v \rho_v (u_{n,v} - u_{n,I}),
\]

where \( u_n \) is the velocity normal to the interface. The normal velocity of the interface is defined as:

\[
u_{n,I} = \mathbf{v}_I \cdot \hat{n} - r_b,
\]

where \( r_b \) is the regression rate of the interface from aluminum vaporization or alumina condensation,

\[
r_b = \frac{\dot{m}''}{\rho_l} = \sum_{i=1}^{N_g} \frac{\dot{\omega}''_i}{\rho_l},
\]

and \( \dot{\omega}''_i \) is the gaseous production rate of species \( i \) due to phase change.

Defining a jump in any variable, \( \Psi \), as:

\[
[\Psi] \equiv \Psi_g - \Psi_l,
\]
using the definition of the mixture density, $\rho_m = \alpha_l \rho_l + \alpha_v \rho_v$, and solving for the jump in normal velocity across the interface, $[u_n]$, gives:

$$[u_n] = \left( \frac{\rho_m}{(1 - \alpha_c)\rho_g} - 1 \right) r_b - \frac{\alpha_c}{1 - \alpha_c} \frac{\rho_c}{\rho_g} r_{accr},$$

(2.65)

where

$$r_{accr} = \min(0, u_{n,c} - u_{n,l} + r_b).$$

(2.66)

Since this model does not account for any stripping or splashing effects at the surface, sub-grid condensed phase alumina droplets are not allowed to leave the surface. Thus, $r_{accr}$ is taken to be non-zero only if particles are impacting the surface.

The first term in the velocity jump represents the Stefan (or blowing) velocity at the surface due to vaporization. The second term represents the velocity jump due to condensed-phase alumina droplet accretion on the liquid interface.

If it is assumed that there are not any vapor bubbles in the liquid phase ($\rho_m = \rho_l$) and there are no droplets in the gas-phase region, then

$$[u_n] = \left[ \frac{1}{\rho} \right] \bar{n}^\nu,$$

(2.67)

which is the classical result for Stefan velocity.

### 2.4.2 Interfacial Normal Momentum Balance

The control volume and free body diagram for the normal momentum balance are shown in Figure 2.6. Neglecting the solids pressure, $p_c$, and performing a momentum balance yields:
\[(1 - \alpha_c) \rho_g u_{n,g}(u_{n,g} - u_{n,l}) + \alpha_c \rho_c u_{n,c}(u_{n,c} - u_{n,l}) - \rho_m u_{n,l}(u_{n,l} - u_{n,l}) = \]
\[(p_l - \sigma_{nn,l}) - (p_g - (1 - \alpha_c)\sigma_{nn,g}) + \frac{1}{A} f_{\sigma_t} \cdot \hat{n}. \quad (2.68)\]

The net surface tension force in the normal direction is:

\[f_{\sigma_t} \cdot \hat{n} A = -\sigma_t \nabla \cdot \hat{n} A = -\sigma_t \kappa_c A, \quad (2.69)\]

where \(\kappa_c\) is the interface curvature (\(\kappa_c = \nabla \cdot \hat{n}\)) and \(\sigma_t\) is the surface tension. Recalling that \(u_{n,l} = u_{n,l} - r_b\), we have:

\[\rho_m r_b [u_n] + \alpha_c \rho_c r_{accr} (u_{n,c} - u_{n,g}) = -[p] + [\alpha_{cont}\sigma_{nn}] - \kappa_c \sigma_t, \quad (2.70)\]

where \(\alpha_{cont}\) is the volume fraction of the continuous phase (i.e., unity in the liquid region and \(1 - \alpha_c\) in the gas region). The above expression provides a relationship for jumps in both pressure and normal deviatoric stress at the interface in terms of phase change, particle accretion, and surface tension. The first term represents the thrust on the surface due to phase change (sometimes called recoil pressure) and the second term represents the momentum contribution from condensed phase droplets impacting the surface.

Assuming no phase change, vapor bubbles, or condensed phase products, the stress condition at the interface reduces to \([p] - [\sigma_{nn}] = -\sigma_t \kappa_c\), which is the classical result for the jump in normal stress due to surface tension. In practice, the jump in normal stress due to surface tension is usually taken to be solely in pressure, which leaves the jump in deviatoric normal stress to be zero. Following this line of thought, we have:

\[[p] = -\kappa_c \sigma_t - \rho_m r_b [u_n] - \alpha_c \rho_c r_{accr} (u_{n,c} - u_{n,g}) \]
\[[2.71]\]

and

\[[\alpha_{cont}\sigma_{nn}] = 0. \quad (2.72)\]

### 2.4.3 Interfacial Tangential Momentum Balance

The control volume and free body diagram for the tangential direction are shown in Figure 2.7. Performing the momentum balance gives:

\[(1 - \alpha_c) \rho_g u_{t,g}([u_n] + r_b) + \alpha_c \rho_c u_{t,c} r_{accr} - \rho_m u_{t,l} r_b = (1 - \alpha_c)\sigma_{nt,g} - \sigma_{nt,l} + \frac{1}{A} f_{\sigma_{net}} \cdot \hat{t}, \quad (2.73)\]
Figure 2.7: Control volume and free body diagram for the tangential momentum balance.

where $u_t$ is the tangential velocity at the interface. The tangential surface tension force is,

$$ f_{σ_t} \cdot \hat{t} = -A \nabla_s σ_t $$

where:

$$ \nabla_s \equiv \nabla - \hat{n} \frac{∂}{∂\hat{n}}. $$

Substituting results from the normal velocity jump and simplifying gives:

$$ [α_{cont} σ_{nt}] = ρ_m r_b [u_t] + α_c ρ_c r_{acrr} (u_{t,c} - u_{t,g}) - \nabla_s σ_t. $$

If there is not any mass exchange between the liquid and gas phase regions the above expression reduces to the classical result for the Marangoni stress, which results in fluid motion induced by surface tension gradients:

$$ [α σ_{nt}] = -\nabla_s σ_t. $$

As particles or droplets become very small, $d < O(20 \mu m)$, enforcing the no-slip condition may not be accurate since the length scale of the droplet, $l_d$, becomes comparable to the mean free path of the gaseous molecules. That is, the Knudsen number, $Kn \equiv λ_{mfp}/l_d$, becomes $O(10^{-1} - 10^0)$. There are various methods of including these effects within the Navier-Stokes equations. One of the simplest methods that requires very few empirical constants is the Maxwell-Smoluchowski partial slip boundary condition [89]:

$$ [u_t] = \frac{2 - \bar{α}}{α} \frac{2μ_g}{ρ_g} \sqrt{\frac{π}{8R_g T_g}} \frac{∂u_t}{∂n} + \frac{3}{4} \frac{μ_g}{ρ_g T_g} \frac{∂T}{∂t}, $$

where $\bar{α}$ is the reflection coefficient (taken to be one), $\hat{n}$ is the normal direction, and $\hat{t}$ is the tangential direction. It is often assumed the accommodation coefficient is unity in lieu of
reliable data or theory to select this number [89]. In usual circumstances the slip velocity is very small. Neglecting the temperature effects and performing a simple scaling analysis with $\rho \sim O(1)$, $\mu \sim O(10^{-5})$, $R_g \sim O(100)$, and $T_g \sim O(1000)$ and normalizing the normal distance, $\hat{n}$, by the particle size reveals:

$$[u_t] \sim 10^{-8} \frac{1}{l_d} \frac{\partial u_t}{\partial \hat{n}},$$

which indicates that velocity slip is negligible unless the droplet length scale is on the order of 1 $\mu$m or there is a very strong shear wave near the interface. If significant amount of slip is present, the jump condition for the total shear stress is unaltered if there is no phase change. If there is mass exchange and the no-slip condition does not hold, then a jump in shear stress is present even if the Marangoni stress is neglected. Physically, the vaporized gas must be accelerated from the liquid tangential velocity to the gas tangential velocity, creating a net change of gas phase momentum.

### 2.4.4 Interfacial Gas-Phase Species Mass Balance

In contrast to the other quantities, the gaseous species mass equations do not exist in the liquid phase. Thus, boundary rather than jump conditions are needed at the interface. A control volume for the surface mass balance of chemical species $i$ is shown in Figure 2.8. In general, a chemical species does not exist in the same form in both liquid and gas phases. Thus, liquid species are not considered in the gas phase species mass balance. However, any
vapor bubbles being exposed due to surface regression add to the species mass balance and should be taken into consideration. The species balance is:

\[
(1 - \alpha_c) \rho_g Y_{i,g}([u] + r_b) + (1 - \alpha_c) J''_i - (1 - \alpha_l) \rho_v Y_{i,v}(r_b) = \alpha_l \dot{\omega}''_i .
\]  

(2.79)

Substituting the velocity jump and the regression rate derived earlier produces a relationship for the diffusion flux at the surface, \( J''_i \), and provides a boundary condition for the mass diffusion fluxes:

\[
(1 - \alpha_c) J''_i = \alpha_l \dot{\omega}''_i + (1 - \alpha_l) \rho_v Y_{i,v} r_b + \alpha_c \rho_c Y_{i,g} r_{acc} - \rho_m Y_{i,g} r_b.
\]  

(2.80)

Unlike the jump conditions derived earlier, the boundary conditions for the species equation at the interface may be written in different forms depending upon the nature of heterogeneous chemical reactions. For example, if the surface chemistry is known, then the above expression is used directly to calculate diffusive flux at the surface.

One special case is diffusion-controlled evaporation, where the evaporation rate is determined by how quickly the Stefan flow and diffusion can carry the vapor away from the surface. For this case, the surface of the liquid is saturated with vapor, (i.e., \( Y_{i,g} = Y_{i,\text{sat}} \)). If it is assumed that evaporation is the only phase change process and there is no accretion of alumina particles, the evaporation mass flux is:

\[
\dot{\omega}''_i = \dot{m}_{\text{evap}} = \frac{J''_i}{1 - Y_{i,\text{sat}}},
\]  

(2.81)

which is the classical result. Although simple, diffusion-limited evaporation will not be assumed. In this work the rate of evaporation from the surface will be calculated using the kinetic theory approach discussed later. Although diffusion-limited evaporation has a very simple form, it poses a problem when using explicit numerical methods. If the diffusion limited assumption is used, it is impossible to separate diffusion from convective processes. Thus, the hyperbolic and diffusive terms in the Navier-Stokes equations should be fully coupled and that the same solver must be used for both wave propagation and diffusion processes. If diffusion and wave propagation can be numerically separated, solvers that work most efficiently for each physical process can be used.
2.4.5 Interfacial Liquid-Phase Species Mass Balance

Since liquid phase species diffusion is neglected in this model, true liquid phase species mass conservation cannot exist at the interface. As shown above, diffusion is needed to balance the convection and surface reaction terms. To rectify this imbalance, a fictitious diffusion term \( J''_{i,l} \) will be used only at the surface. Considering the species mass balance shown in Figure 2.9, the fictitious diffusion flux, \( J''_{i,l} \), can be defined as:

\[
\alpha_l J''_{i,l} = \alpha_c \rho_c u_{n,c} Y_{i,c} r_{accr} - \alpha_l \rho_l Y_{i,l} r_b - \alpha_l \dot{\omega}''_{i,l}.
\]  
(2.82)

Summing the fictitious diffusion flux over all liquid species reveals that

\[
\alpha_l \sum J''_{i,l} = \alpha_c \rho_c r_{accr},
\]  
(2.83)

which is the net mass of particles being absorbed by the liquid. If there is only one liquid-phase species, this ad-hoc step is not necessary.

2.4.6 Interfacial Energy Balance

Performing an energy balance on the control volume shown in Figure 2.10 gives:
Figure 2.10: Control volume for energy balance across a gas/liquid interface.

\[
\begin{align*}
\rho_m H_m r_b - (1 - \alpha_c) \rho_g H_g (u_n + r_b) &= -\alpha_c \rho_c r_{accr} + \\
\dot{q}_{\text{cond},l}'' - (1 - \alpha_c) \dot{q}_{\text{cond},g}'' &= (1 - \alpha_c) \sigma_{nn,l} u_{n,l} - \sigma_{nt,l} u_{t,l} + (1 - \alpha_c) \dot{q}_{\text{diff},g}'' + (1 - \alpha_c) \sigma_{nn,l} u_{n,l} - \sigma_{nt,l} u_{t,l} = 0, \\
\end{align*}
\]

where \( H \) is the specific stagnation enthalpy including the chemical energy. Solving for the conduction heat flux jump and simplifying gives:

\[
\begin{align*}
[\dot{q}_{\text{cond}}] &= \rho_m r_b (H_m(T_m) - H_g(T_g)) + \alpha_c \rho_c r_{accr} (H_c(T_c) - H_g(T_g)) + \\
[\alpha_{\text{cont}} \sigma_{nn} u_n] + [\alpha_{\text{cont}} \sigma_{nt} u_t] &= (1 - \alpha_c) \dot{q}_{\text{diff},g},
\end{align*}
\]

where \( \dot{q}_{\text{diff}} \) is the net heat flux due to species mass diffusion.

If it is assumed that only one liquid species is present, the heat flux from species mass diffusion and work due to the deviatoric stresses are neglected, and there are not any condensed-phase particles we have:

\[
[\dot{q}_{\text{cond}}] = \dot{m}'' (H_l - H_g),
\]

which is a classical result stating that the latent heat liberated due to vaporization at the surface is balanced by a jump in surface heat flux.

Similar to the tangential velocity, if the droplet is very small or a strong shock wave impacts the interface there may be a temperature jump at the surface. One simple method
to calculate the temperature jump $[T]$ is [89]:

$$[T] = \frac{2 - \bar{\sigma}}{\bar{\sigma}} \frac{2 \gamma}{\gamma + 1} \mu_g \sqrt{\frac{\pi}{8R_g T \Pr_g}} \frac{1}{\bar{n}} \partial T,$$  

where $\bar{\sigma}$ is the accommodation coefficient (taken to be unity), and $\Pr_g$ is the Prandtl number of the gas.

### 2.4.7 Phase Change at an Interface

#### 2.4.7.1 Evaporation/Condensation

One method to calculate the mass transfer due to vaporization/condensation at an interface is via the Schrage equation [10],

$$\dot{m}_{\text{evap},i}'' = \frac{2c}{2 - c} \sqrt{\frac{Mw_i}{2\pi R_g T}} (p_{\text{sat},i} - p_i)$$  

where $c$ is the condensation or evaporation depending on the nature of the phase change. The condensation coefficient represents the ratio of the number of molecules absorbed by the liquid to the number of molecules that impacted the surface. Due to vapor molecules reflecting from the surface, the condensation coefficient is normally less than one. The evaporation coefficient represents the ratio of the number of liquid molecules transferred to the gas phase to the total number of molecules emitted from the liquid phase. A schematic diagram of the condensation and evaporation mechanisms are shown in Figure 2.11. Measurements of the condensation coefficient of water shows about three decades of data scatter, with values ranging between unity and 0.001 [111]. Nagayama and Tsuruta [112] used molecular dynamic calculations and developed an overall expression to estimate the condensation coefficient, which is given by:

$$c = \left[ 1 - \left( \frac{\rho_g}{\rho_l} \right)^{1/3} \right] \exp \left( -\frac{1}{2(\rho_l/\rho_g)^{1/3} - 2} \right).$$  

In its original form the Schrage-Knudsen equation is only valid for pure liquids; however, in the case of multi-component liquid mixtures the net rate of phase change can be approximated by:

$$\dot{m}_{\text{evap},i}'' = \frac{2c}{2 - c} \sqrt{\frac{Mw_i}{2\pi R_g T}} (X_{i,l}p_{\text{sat},i} - p_i).$$  

(2.90)
The Schrage equation was derived using the kinetic theory of gases and assuming that the interface is planar. If the surface is strongly curved, the saturation pressure used in the Schrage equation should be modified \[96\] by:

$$p_{\text{sat,cor}} = p_{\text{sat,planar}} \exp \left( \frac{2 \sigma_t M_w}{r_{\text{curv}} R_u p_l T} \right), \quad (2.91)$$

where \(r_{\text{curv}}\) is the radius of curvature of the interface and \(p_{\text{sat,planar}}\) is from measured data. The saturation pressure of liquid Al is given by:

$$p_{\text{sat}}(Pa) = \exp \left[ 36.547 - \frac{39033}{T} - 1.3981 \ln(T) + 6.7839 \times 10^{-9}T^2 \right], \quad (2.92)$$

where the temperature is in degree Kelvin.

### 2.4.7.2 Heterogeneous Surface Kinetics

Data on heterogeneous chemistry that is directly usable for numerical modeling purposes is scarce. In fact, only one paper by Steinberg et al. \[19\] gave both the form and the parameters
for a global heterogeneous reaction of Al with GOx. Their results indicate that the overall consumption rate of Al for their experiments can be expressed by:

$$\dot{\omega}''_{Al,i} (g/m^2s) = -\frac{0.102 p_{O_2}(MPa)}{1 + 0.186 p_{O_2}(MPa)}.$$  \hspace{1cm} (2.93)

The authors did not mention what products this heterogeneous reaction produces, they were only interested in the regression rate of Al. With this ambiguity, there are two basic choices; the liquid Al can react with oxygen to produce gas phase intermediate species, such as AlO, or the overall heterogeneous reaction produces liquid alumina on the surface directly.

Another option to calculate heterogeneous reaction rates is to use kinetic theory. If this method is adopted, the heterogeneous reaction rate would be equated to the rate that gas-phase reactants are impacting the surface, $J_i$. From kinetic theory, the rate at which molecules strike a surface is [35]:

$$J_i = \gamma_i N_i \sqrt{\frac{k_B T}{2\pi m_{molec}}}.$$  \hspace{1cm} (2.94)

where $\gamma_i$ is the sticking coefficient, $N_i$ is the number density of species $i$, and $m_{molec}$ is the mass of the molecule hitting the surface. In lieu of any other information, the sticking coefficient could be taken as unity.

Without any reliable surface reaction mechanisms and the completely different physical setup of Steinberg et al. [19], surface reactions are not considered in this work. As mentioned in Chapter 1, at high pressures the boiling point of Al can exceed the flame temperature and surface reactions dominate and need to be considered. If the model developed in this work is used on transitionally-sized Al droplets—where both kinetic and diffusion effects are important—in the future, surface reactions will also have to be reconsidered.
3.1 Compressible Navier-Stokes Equations and Operator Splitting Techniques

A system of conservation laws for a compressible reacting gas in two dimensions is:

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \eta \frac{\partial \mathbf{G}_r}{\partial y} + \frac{1}{y^{\eta}} \frac{\partial y^{\eta} \mathbf{G}_v}{\partial y} = \mathbf{S},
\]

(3.1)

where

\[
\mathbf{U} = \begin{bmatrix}
\rho Y_1 \\
\vdots \\
\rho Y_{N_g} \\
\rho u \\
\rho v \\
\rho E
\end{bmatrix}, \quad
\mathbf{F} = \begin{bmatrix}
\rho u Y_1 \\
\vdots \\
\rho u Y_{N_g} \\
\rho u^2 + p \\
\rho uv \\
u(\rho E + p)
\end{bmatrix}, \quad
\mathbf{G} = \begin{bmatrix}
\rho v Y_1 \\
\vdots \\
\rho v Y_{N_g} \\
\rho vu \\
\rho v^2 + p \\
v(\rho E + p)
\end{bmatrix}, \quad
\mathbf{G}_r = \begin{bmatrix}
\rho v Y_1 \\
\vdots \\
\rho v Y_{N_g} \\
\rho vu \\
\rho v^2 \\
v(\rho E + p)
\end{bmatrix},
\]
\[
\mathbf{F}_v = \begin{bmatrix}
-J_{x,1} \\
\vdots \\
-J_{x,N_g}
\end{bmatrix}, \quad \mathbf{G}_v = \begin{bmatrix}
-J_{y,1} \\
\vdots \\
-J_{y,N_g}
\end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix}
\dot{\omega}_1 \\
\vdots \\
\dot{\omega}_{N_g}
\end{bmatrix},
\]

and \( \eta \) is the coordinate system selector given by Eq. (2.9). Directly coupling all of the physical processes in a system of conservation laws together is usually impractical due to a disparity in time scales between various physical processes. The method of fractional steps (also called operator-split methods) splits the integration of Eq. (3.1), into a series of steps that effectively decouple the physical processes and/or spatial direction. This allows each process to be integrated using numerical methods that are most suitable. For example, the general 2-D balance laws can be split into hyperbolic, parabolic, and inhomogeneous steps.

\[
\begin{align*}
\frac{\partial \mathbf{U}}{\partial t} &= -\frac{\partial \mathbf{F}}{\partial x} - \frac{\partial \mathbf{G}}{\partial y} - \eta \frac{\partial \mathbf{G}_x}{\partial y}, \\
\frac{\partial \mathbf{U}}{\partial t} &= -\frac{\partial \mathbf{F}_v}{\partial x} - \frac{1}{y} \frac{\partial y^n \mathbf{G}_v}{\partial y}, \\
d\mathbf{U}/dt &= \mathbf{S}.
\end{align*}
\]

Godunov splitting [113], which is first order accurate, integrates \( \mathbf{U} \) from time \( n \) to \( n + \Delta t \) by:

\[
\mathbf{U}^{n+\Delta t} = \mathbf{S}^{\Delta t} \mathbf{P}^{\Delta t} \mathbf{H}^{\Delta t}(\mathbf{U}^n),
\]

where \( \mathbf{H}^{\Delta t}, \mathbf{P}^{\Delta t}, \mathbf{S}^{\Delta t} \) represent operators to integrate the hyperbolic, parabolic, and inhomogeneous step respectively for a time step of \( \Delta t \). One problem with the splitting method given by Eq. (3.5) is that it is formally first-order accurate [113, 114]. One of the most commonly used second-order fractional step methods is Strang splitting:

\[
\mathbf{U}^{n+2\Delta t} = \mathbf{H}^{\Delta t} \mathbf{P}^{\Delta t} \mathbf{S}^{2\Delta t} \mathbf{P}^{\Delta t} \mathbf{H}^{\Delta t}(\mathbf{U}^n),
\]

which is really two Godunov steps used in sequence with the order of the operators permuted. In multiple dimensions, spatial direction as well as physical processes are often split. If the
hyperbolic integrator is split into a dimension-by-dimension basis we have:

\[ \mathbf{U}^{n+2\Delta t} = \mathcal{H}_x^{\Delta t} \mathcal{H}_y^{\Delta t} \mathcal{P}_{xy}^{2\Delta t} \mathcal{S}_{xy}^{2\Delta t} \mathcal{P}_{xy}^{\Delta t} \mathcal{S}_{xy}^{\Delta t} \mathcal{H}_x^{\Delta t} \mathcal{H}_y^{\Delta t} \mathcal{(U^n)}. \]  

(3.7)

The order of the operators is not important for any splitting method; however, with Strang splitting order of the operators must be permuted after the middle step. It would also be unwise to put the operator with the most restrictive time step as the middle operator. Consider the two-dimensional Euler equations split by \( \mathbf{U}^{n+2\Delta t} = \mathcal{H}_x^{\Delta t} \mathcal{H}_y^{\Delta t} \mathcal{H}_x^{\Delta t} \mathcal{(U^n)}. \) This requires the Courant number to be less than 0.5 due to the time step of \( 2\Delta t \) for y-direction. Leveque [114] points out that although Strang splitting is formally second order, in practice the differences between calculated results using either method are often very small. Thus, the choice of which method to use is often made by computational efficiency.

The integration of the hyperbolic, parabolic, and inhomogeneous portions will be discussed in turn.

### 3.2 Integration of the Hyperbolic Step

The solution methods described in this section are used to solve the hyperbolic conservation law:

\[ \frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0. \]

(3.8)

What makes integrating the general hyperbolic conservation law challenging is that the conserved variables cannot be integrated in a straight-forward upwind manner since wave information can propagate against the flow. The propagation velocity of the waves can be determined by calculating the eigenvalues, \( \lambda \), of the flux Jacobian, \( \mathbf{A} \equiv \frac{\partial (\mathbf{F}(\mathbf{U}))}{\partial \mathbf{U}}. \) It must be noted that the methods presented in this section are only valid if the conservation laws are strictly hyperbolic, that is all the eigenvalues of \( \mathbf{A} \) are real and distinct and all eigenvectors are linearly independent. If the eigenvalues are all real but not distinct, the conservation laws are weakly hyperbolic. Weakly hyperbolic systems, such as the multi-component Euler equations, require some modification to handle contact surfaces correctly. When one or more of the eigenvalues are imaginary, the conservation law is no longer hyperbolic and the methods described in this section are no longer valid.
3.2.1 Godunov Based Methods

Many modern high-resolution finite volume schemes are based on Godunov’s scheme, which splits the domain into a series of piecewise constant states where the generalized Riemann problem:

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0
\]

is solved exactly at each cell face located at \( x = x_{i+1/2} \) and then re-averaged into the cells as shown in Figure 3.1. Godunov’s method can also be viewed as discretizing the hyperbolic conservation law in a manner similar to the finite volume method:

\[
U_{i}^{n+1} = U_{i}^{n} - \frac{\Delta t}{\Delta x} (F_{i+1/2} - F_{i-1/2}),
\]

where the edge fluxes are obtained from the solution to the Riemann problem at \( 1/2\Delta t \) at each cell face as shown in Figure 3.2.

Modern techniques use high-order interpolation methods to determine the left and right states at the cell edge \( U_L \) and \( U_R \). When using high-order interpolation, care must be taken...
to ensure that new extrema are not introduced. Two popular methods for performing the interpolation are the Monotone Upstream-centered Scheme for Conservation Laws (MUSCL), which are usually second- or third-order accurate in space and the Weighted Essentially Non-Oscillatory (WENO) class of schemes are up to 17th order accurate in smooth regions. Details of the WENO and MUSCL interpolation methods are given in Appendix B.

Modern techniques follow the second interpretation of Godunov’s method and use Riemann problems defined by the high-order interpolation to form a numerical flux vector at the cell edges as shown in Figure 3.2. While powerful, Godunov-based methods—often called Flux Difference Splitting (FDS)—require the solution of Riemann problems at each cell face, which can be very expensive. Another problem using Godunov’s method is that exact Riemann solvers have only been developed for simplified equations of state such as the ideal gas law or the stiffened equation of state. To overcome some of these problems, a variety of approximate Riemann solvers have been developed.

### 3.2.1.1 HLLC Approximate Riemann Solver

One of the most popular approximate Riemann solvers is the Harten, Lax, van Leer with Contact (HLLC) solver. Details on the derivation of the HLLC Riemann solver can be found in Toro et al. [115], Toro [113], and Johnson and Colonius [116]. The HLLC flux is defined
by:

\[ F_{i+1/2}^{\text{HLLC}} = \begin{cases} 
  F_L & \text{if } 0 \leq s_L \\
  F_L + s_L(U_L^s - U_L) & \text{if } s_L \leq 0 \leq s^* \\
  F_R + s_R(U_R^s - U_R) & \text{if } s^* \leq 0 \leq s_R \\
  F_R & \text{if } 0 \geq s_R,
\end{cases} \quad (3.11) \]

where

\[ s^* = \frac{p_R - p_L + \rho_L u_L (s_L - u_L) - \rho_R u_R (s_R - u_R)}{\rho_L (s_L - u_L) - \rho_R (s_R - u_R)}. \quad (3.12) \]

There are many different methods to calculate the fastest and slowest signal speeds, \( s_L \) and \( s_R \), for the HLLC scheme including:

\[ \begin{align*}
  s_L &= u_L - c_L & s_R &= u_R + c_R \\
  s_L &= \max(u_L - c_L, u_R - c_R) & s_R &= \max(u_L + c_L, u_R + c_R) \\
  s_L &= \max(\bar{u} - \bar{c}, u_L - c_L) & s_R &= \max(\bar{u} + \bar{c}, u_R + c_R),
\end{align*} \quad (3.13) \]

where \( \bar{u} \) and \( \bar{c} \) refer to the Roe averaged velocity and sound speed, respectively [see Eq. (3.21) for the definition of Roe averaged variables for the 1-D Euler equations].

In two dimensions, the star state is defined as:

\[ U_k^* = \frac{s_k - u_k}{s_k - s^*} \left( \begin{array}{c}
  \rho_k \\
  \rho_k s^* \\
  \rho_k v_k \\
  \rho_k E_k + \rho_k (s^* - u_k) \left( s^* + \frac{p_k}{\rho_k (s_L - u_L)} \right)
\end{array} \right), \quad (3.16) \]

where \( k \) refers to either the left or right interpolated state.

3.2.1.2 Rusanov Flux

The Rusanov flux [113] is simpler, but much more dissipative than the HLLC Riemann solver. The Rusanov flux is given by:

\[ F_{i+1/2} = \frac{1}{2} [F(U_L) - F(U_R)] - \frac{S^+}{2} (U_R - U_L), \quad (3.17) \]
where
\[ S^+ = \max(|u_L| + c_L, |u_R| + c_R). \] (3.18)

**3.2.2 Flux Vector Splitting**

Rather than solving the Riemann problem at each interface, flux vector splitting (FVS) splits the flux vector into positive and negative directions via
\[ F = F^+ + F^- \] (3.19)

and
\[ \frac{\partial F}{\partial x} = \frac{\partial F^+}{\partial x} + \frac{\partial F^-}{\partial x}, \] (3.20)
where \( F^+ \) is guaranteed to be in the positive direction and \( F^- \) is guaranteed to be in the negative direction. Splitting the flux into this fashion allows the use of standard upwind finite difference operators to compute the flux derivative. There are many methods to split the fluxes such as van Leer splitting and Steger-Warming splitting [113], and some have been extended to real gases [117, 118].

A current method developed by Balsara and Shu [119] uses the WENO class of schemes for discretization and characteristic-based flux splitting. The characteristics of a hyperbolic system are the linearized and decoupled scalar waves of the conservation laws. The first step in their procedure is to estimate the left and right eigenvectors of the flux Jacobian, \( \textbf{L} \) and \( \textbf{R} \), at the cell edges.

Since the primitive variables (\( \rho, u, p, T \)) are needed to form the eigenvalues are not initially known at the cell edges, Roe averaged variables [120] are utilized to estimate the eigenvectors:
\[ \tilde{u} \equiv \frac{\sqrt{\rho_i} u_i + \sqrt{\rho_{i+1}} u_{i+1}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}, \]
\[ \tilde{H} \equiv \frac{\sqrt{\rho_i} h_{t,i} + \sqrt{\rho_{i+1}} h_{t,i+1}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}, \]
\[ \tilde{c} \equiv \sqrt{(\gamma - 1) \left[ \tilde{H} - \frac{\tilde{u}^2}{2} \right]}. \] (3.21)

Using the left and right eigenvectors for cell edge \( i+1/2 \), the flux vector, \( \textbf{F} \) is transformed into upwind, \( \textbf{F}^+ \), and downwind, \( \textbf{F}^- \), characteristic-based fluxes for every cell in the numerical
stencil using Local Lax-Friedrichs flux splitting.

\[
F_{i+\frac{1}{2}}^+ = \frac{L_{i+\frac{1}{2}} \cdot (F_{i+k} + \hat{\lambda}_{i+\frac{1}{2}} \cdot U_{i+k})}{2}; \quad k = i - N_u, \ldots, i + N_d
\]

\[
F_{i+\frac{1}{2}}^- = \frac{L_{i+\frac{1}{2}} \cdot (F_{i+k} - \hat{\lambda}_{i+\frac{1}{2}} \cdot U_{i+k})}{2}; \quad k = i - N_d, \ldots, i + 1 + N_d
\]

where \(N_u\) is the number of grid points in the stencil upstream of the cell edge and \(N_d\) is the number of grid points in the stencil downstream of the cell edge. The maximum wave speed array, \(\hat{\lambda}_{i+\frac{1}{2}}\), is defined by:

\[
\hat{\lambda}_{i+\frac{1}{2}} = \chi \text{diag} \left( \begin{array}{c}
\max(\{|u - c|_{i-N_u}, \ldots, |u - c|_{i+N_u}\}) \\
\max(\{|u|_{i-N_u}, \ldots, |u|_{i+N_u}\}) \\
\max(\{|u + c|_{i-N_u}, \ldots, |u + c|_{i+1+N_u}\})
\end{array} \right)
\]

where \(\chi\) is a parameter (set to 1.3 unless otherwise noted) to control artificial dissipation. After the fluxes are split into upwind and downwind direction, they are interpolated to the cell edges using the high-order interpolation methods described in Appendix B.

The final step of the flux evaluation procedure is to combine the upwind and downwind interpolated characteristic-based fluxes and project them back to the physical system:

\[
F_{i+\frac{1}{2}} = R_{i+\frac{1}{2}} \cdot \left( F_{i+\frac{1}{2}}^+ + F_{i+\frac{1}{2}}^- \right).
\]

Although complicated and fairly expensive, this technique produces very accurate results that are relatively free of spurious oscillations when shock waves reflect off walls or collide.

### 3.2.3 Advection Upstream Splitting Methods

The Advection Upstream Splitting Method (AUSM) developed by Liou and Steffen [121] is a method that combines the ideas of both Godunov-type methods and FVS. AUSM splits the flux at the cell edge into convective and pressure fluxes:

\[
F_{1/2} = F_{1/2}^c + p_{1/2},
\]

where

\[
F_{1/2}^c = \hat{m}_{1/2}'' \psi_{L/R},
\]

\[
F_{1/2}^p = \hat{m}_{1/2}'' \psi_{L/R}.
\]
and \( \mathbf{p} \) is a flux vector that contains pressure for the momentum equation. The vector \( \psi \) represents the variables which are advected with the flow such as mass fraction, velocity, and stagnation enthalpy.

Rather than splitting the fluxes at the grid points as with FVS, AUSM forms the fluxes at the cell edges by the splitting and recombining them based on the left and right interpolated variables. AUSM has been extended to the AUSM+ scheme [122] and the AUSM+-up [123] to overcome some of the shortcomings of the original AUSM method.

Before the AUSM+–up scheme is described, several necessary functions that are used to split the Mach number and the pressure at the cell edge are given:

\[
\mathcal{M}_1^\pm(M) = \frac{1}{2} (M \pm |M|),
\]

\[
\mathcal{M}_2^\pm(M) = \pm \frac{1}{4} (M \pm 1)^2,
\]

\[
\mathcal{M}_4^\pm(M) = \begin{cases} 
\mathcal{M}_1^\pm(M) & \text{if } |M| \geq 1 \\
\mathcal{M}_2^\pm(M)[1 \mp 16\beta \mathcal{M}_2^\pm(M)] & \text{if } |M| < 1,
\end{cases}
\]

\[
\mathcal{P}_5^\pm(M) = \begin{cases} 
\mathcal{M}_1^\pm(M) & \text{if } |M| \geq 1 \\
\mathcal{M}_2^\pm(M)[(\pm 2 - M) \mp 16\alpha M \mathcal{M}_2^\pm(M)] & \text{if } |M| < 1,
\end{cases}
\]

where \( \alpha \) and \( \beta \) are constants to be determined later.

After performing the edge interpolation from the left and right, the numerical Mach number of the left and right interpolated states, \( M_L \) and \( M_R \), are determined from the numerical speed of sound at the interface, \( c_{1/2} \). The speed of sound at the interface is defined by:

\[
c_{1/2} = \min(\hat{c}_L, \hat{c}_R),
\]

where

\[
\hat{c}_L = \frac{c^2}{\max(c^*, u_L)},
\]

\[
\hat{c}_R = \frac{c^2}{\max(c^*, -u_R)},
\]
and \( c^* \) is critical speed of sound (the speed of sound for a fluid accelerated isentropically from rest to the sonic condition). The critical speed of sound for an ideal gas is:

\[
c^*^2 = 2H \frac{\gamma - 1}{\gamma + 1}. \tag{3.34}
\]

Next, the parameters \( \bar{M} \), \( M_o \), and \( f_a \) are calculated:

\[
\bar{M}^2 = \frac{u_L^2 + u_R^2}{2c_{1/2}^2}, \tag{3.35}
\]

\[
M_o^2 = \min \left[ 1, \max \left( \bar{M}^2, M_{\infty}^2 \right) \right], \tag{3.36}
\]

\[
f_a = M_o(2 - M_o), \tag{3.37}
\]

where \( M_{\infty} \) is a representative Mach number of the flow (zero for the shock-tube type situations in this work). The Mach number at the cell face, \( M_{1/2} \), is:

\[
M_{1/2} = M_4^+(M_L) + M_4^-(M_R) - \frac{2K_p}{f_a} \max(1 - \sigma \bar{M}^2, 0) \frac{p_R - p_L}{(\rho_L + \rho_R)c_{1/2}^2}, \tag{3.38}
\]

where \( K_p \) and \( \sigma \) are adjustable constants between zero and one.

Using the above parameters, the split mass flux is:

\[
\dot{m}_{1/2}'' = c_{1/2}M_{1/2} \begin{cases} 
\rho_L & \text{if } M_{1/2} \geq 0 \\
\rho_R & \text{if } M_{1/2} < 0,
\end{cases} \tag{3.39}
\]

and the split pressure is:

\[
p_{1/2} = \mathcal{P}_5^+(M_L)p_L + \mathcal{P}_5^-(M_R)p_R - K_u f_a c_{1/2} \mathcal{P}_5^+(M_L)\mathcal{P}_5^-(M_R)(\rho_L + \rho_R)(u_R - u_L), \tag{3.40}
\]

where \( K_u \) is a constant between zero and one. The final AUSM flux used for the integration of the conservation law is:

\[
\mathbf{F}_{1/2} = \mathbf{p}_{1/2} + \dot{m}_{1/2}'' \begin{cases} 
\psi_L & \text{if } \dot{m}_{1/2}'' \geq 0 \\
\psi_R & \text{if } \dot{m}_{1/2}'' < 0,
\end{cases} \tag{3.41}
\]
where $\mathbf{p}_{1/2}$ is a pressure flux vector that is non-zero only for the moment equation (e.g., for the flux in the x-direction of the 2-D single-component Euler equations $\mathbf{p}_{1/2} = (0, p_{1/2}, 0, 0)^T$) and $\psi$ is the vector of the passively advected scalars (e.g., $\psi = (1, u, v, H)^T$ for 2-D Euler equations).

The constant $\alpha$ used in the $M_4$ function is defined by:

$$\alpha = \frac{3}{16} (-4 + 5 f_a^2). \quad (3.42)$$

The other constants, unless otherwise noted, are the values recommended by Liou [123], $\beta = 1/8$, $K_p = 0.25$, $K_u = 0.75$, and $\sigma = 1.0$.

There have been many variants to the AUSM+ scheme including the AUSMPW+ [124], Low Diffusion Flux Splitting (LDFSS) for real fluids [125], LDFSS for dense gas-solid flows [126], and an AUSM variant for compressible two-phase flow [127] to name a few. One group [83] even took advantage of that fact that AUSM is a combination of Godunov-type methods and FVS and used the HLLC approximate Riemann solver to calculate the mass flux through the cell edge, but retained the pressure splitting of AUSM. Most of these variants differ in how the Mach number splitting, pressure splitting, and interface sound speed are calculated. In the case of two-phase cavitating flows the critical speed of sound is difficult to calculate, in place of this Edwards et al. [125] based the numerical sound speed on the acoustic impedance of the two-phase mixture:

$$c_{1/2} = \sqrt{\frac{(\rho_L c_L^2) + (\rho_R c_R^2)}{\rho_L + \rho_R}}. \quad (3.43)$$

### 3.2.3.1 Simple Low-Dissipation AUSM

A recent extension to AUSM is the Simple Low-dissipation AUSM 2 (SLAU2) scheme of Kitamura and Shima [128]. The mass flux for SLAU2 is given by:

$$m''_{1/2} = \frac{1}{2} \left[ \rho_L (U_{n,L} + |\bar{U}_n|^L) + \rho_R (U_{n,R} + |\bar{U}_n|^R) - \frac{\chi}{c_{1/2}} (P_R - P_L) \right], \quad (3.44)$$
and the split pressure is:

\[
p_{1/2} = \frac{1}{2} \left[ p_L + p_R + \left( P_5^+ (M_L) - P_5^- (M_L) \right) (p_L - p_R) + \sqrt{\frac{u_L^2 + v_L^2 + u_R^2 + v_R^2}{2}} \left( P_5^+ (M_L) + P_5^- (M_R) - 1 \right) (\rho_L + \rho_R) c_{1/2} \right],
\]

(3.45)

where

\[
\chi = (1 - \hat{M})^2, \quad \hat{M} = \min \left[ 1, \frac{1}{c_{1/2}} \sqrt{\frac{u_L^2 + v_L^2 + u_R^2 + v_R^2}{2}} \right],
\]

\[
M_{L,R} = \frac{U_{n,L,R}}{c_{1/2}}, \quad U_{n,L,R} = u\hat{n}_x + v\hat{n}_y,
\]

\[
|\vec{U}_n|^{L,R} = (1 - g)|\vec{U}_n| + g|U_{n,L,R}|, \quad g = - \max[\min(M_L, 0), -1] \min[\max(M_R, 0), 1],
\]

and

\[
|\vec{U}_n| = \frac{\rho L |U_{n,L}| + \rho R |U_{n,R}|}{\rho L + \rho R}.
\]

SLAU2 has been shown to provide sufficient dissipation to minimize shock anomalies, such as pressure waves generated transverse to shock waves, but still perform very well for boundary layer flows [128].

### 3.2.4 Rotated Riemann Solvers

When using higher-order methods, anomalies and transverse oscillations [128] can form near stationary or slowly-moving normal shock waves and produce oscillations. A recent analysis by Pandolfi and D’Ambrosio [129] showed that the carbuncle instability and its related anomalies are introduced by any flux scheme that explicitly accounts for the presence of the middle contact wave. If the rotated Riemann solver of Huang et al. [130] is utilized the effect of the multidimensional shock anomalies can be reduced significantly. The flux vector, \( \mathbf{F} \), near shock waves is calculated by evaluating the flux vector at two orthogonal directions at the cell face:

\[
\mathbf{F} = \alpha_1 F_{AUSM}(\mathbf{n}_1) + \alpha_2 F_{AUSM}(\mathbf{n}_2).
\]

(3.46)

The normal vectors \( \mathbf{n}_1, \mathbf{n}_2 \) are:

\[
\mathbf{n}_1 = \text{sgn}(\Delta \mathbf{v} \cdot \mathbf{n}) \frac{\Delta \mathbf{v}}{\|\Delta \mathbf{v}\|} \quad \text{and} \quad \mathbf{n}_2 = \frac{(\mathbf{n}_1 \times \mathbf{n}) \times \mathbf{n}_1}{\| (\mathbf{n}_1 \times \mathbf{n}) \times \mathbf{n}_1 \|},
\]

(3.47)
where $\mathbf{n}$ is the outward normal vector of the cell face, $\alpha_1 = \mathbf{n} \cdot \mathbf{n}_1$, and $\alpha_2 = \mathbf{n} \cdot \mathbf{n}_2$. The direction of the rotated Riemann solver is based on the interpolated velocity field where

$$\Delta \mathbf{v} = \langle u_R - u_L, v_R - v_L \rangle. \quad (3.48)$$

The rotated Riemann solver is only activated if $\|\Delta \mathbf{v}\| > 0.1$ and $\alpha_2 > \epsilon_{\text{rot}}$, otherwise standard AUSM$^+$-up scheme is used. The parameter $\epsilon_{\text{rot}}$ is set to 0.5 unless otherwise noted.

Figure 3.3 shows that the rotated Riemann solver significantly decreases transverse shock anomalies, where the exact solution is a vertical line representing the shock wave with out any fluctuations. Increasing the AUSM dissipation parameters has a much smaller effect on reducing the transverse shock anomalies.

### 3.2.5 ODE Integrators for Hyperbolic Problems

One of the most popular methods for discretizing Eq. (3.8) is to use the method of lines, where the spatial discretization is performed as discussed above but the time derivative is left
intact. This produces a system of ODEs that can be integrated using any number of methods. Since wave propagation processes are of interest and a total time of the calculation is on the order of 10 µs, explicit methods will be used for their generality and ease of implementation. In this work a third-order-accurate three-stage low storage strong stability preserving Runge-Kutta (RK3) method is used unless otherwise noted. A three-stage scheme to advance

$$\frac{dQ}{dt} = \mathcal{L}(Q,t)$$  \hspace{1cm} (3.49)

from time step $n$ to $n + 1$, is as follows:

$$Q^{(1)} = Q^n + \Delta t \mathcal{L}(Q^n, t^n)$$

$$Q^{(2)} = \frac{3}{4} Q^n + \frac{1}{4} \left[ Q^{(1)} + \Delta t \mathcal{L}(Q^{(1)}, t^n + \Delta t) \right]$$  \hspace{1cm} (3.50)

$$Q^{n+1} = \frac{1}{3} Q^n + \frac{2}{3} \left[ Q^{(2)} + \Delta t \mathcal{L}(Q^{(2)}, t^n + \frac{\Delta t}{2}) \right].$$

Second order Runge-Kutta (RK2) is also a popular method:

$$Q^{(1)} = Q^n + \Delta t \mathcal{L}(Q^n, t^n)$$

$$Q^{(n+1)} = \frac{1}{2} Q^n + \frac{1}{2} \left[ Q^{(1)} + \Delta t \mathcal{L}(Q^{(1)}, t^n + \frac{\Delta t}{2}) \right].$$  \hspace{1cm} (3.51)

The time step used in this work is based on the Courant-Friedrichs-Lewy (CFL) criterion

$$\text{CFL} = \max \left( \frac{(|u_d| + c) \Delta t}{\Delta x_d} \right)$$  \hspace{1cm} (3.52)

where $\Delta x_d$ is the grid spacing in the d-direction (x or y), $\Delta t$ is the time-step size, and $u_d$ is the velocity in the d-direction.

### 3.2.6 Flux Evaluation for Multi-component Gases

In recent years several schemes have been proposed for calculating compressible multi-component flows [77, 78, 131–133] and more recently a Runge-Kutta Discontinuous Galerkin approach has been proposed [134]. Most of these methods are quasi-conservative—with the exception of the compact-central-differencing method of Kawai and Terashima [132]—and abandon strict conservation near material interfaces. One of the only methods available in
open literature that has been demonstrated with mixtures of non-calorically perfect gases [i.e., $\gamma = \gamma(T, Y_i)$] is the double-flux model of Billet and Abgrall [77], which is based on the quasi-conservative technique developed by Abgrall and Karni [135]. Using the double-flux model to advect the hydrogen bubble does not produce any temperature, pressure, or velocity oscillations as shown in the calculated results from the present scheme (see Figure 3.4b). If left unchecked, the unphysical pressure oscillations and temperatures spikes produced by fully conservative methods may even halt the calculation in severe cases. Even though the compact-central-differencing method of Kawai and Terashima [132] could likely be extended to mixtures of non-calorically perfect gases, block structured Adaptive Mesh Refinement (AMR) is used in this work, which makes using compact-central differencing methods cumbersome. Thus, the double flux model is adopted in this work.

The first step in the double flux model is to evaluate the specific heats for each species in linear interpolation tables, which are formed at the start of the calculation. If $T_m < T < T_{m+1}$ the constant-pressure specific heat of species $i$ is:

$$C_{p_i}(T) = a_i^m T + b_i^m,$$

(3.53)
where \( m \) is the temperature interval. The specific total energy of the mixture is calculated in a form similar to a constant property single-component ideal gases:

\[
E = h_0^m + \frac{p}{\rho(\gamma - 1)} + \frac{u^2 + v^2}{2},
\]

where

\[
h_0^m = \sum_{i=1}^{N} Y_i (\tilde{h}_{i0}^m - \tilde{b}_i^m T_m), \quad \tilde{h}_{i0}^m = h_{fi}^0 + \sum_{k=1}^{m} \left( \int_{T_k}^{T_{k-1}} (a_i^k s + b_i^k) ds \right), \quad \tilde{b}_i^m = \frac{a_i^m}{2} (T + T_m) + b_i^m.
\]

Billet and Abgrall [77] showed that pressure and velocity of a material interface is preserved if \( \gamma \) and \( \rho h_0^m \) are frozen in each cell for the entire time step. Thus, the gas mixture in each computational cell is treated as its own constant property single-component ideal gas. To achieve this, the flux at cell edge \( i + 1/2 \) must be calculated twice, once for the cell on the left using \( \gamma_i \) and \( \rho h_0^m \), and a second time for the cell on the right using \( \gamma_{i+1} \) and \( \rho h_0^m \).

The flux gradient in the x-direction for computational cell \( i \) is:

\[
\frac{\partial F_i}{\partial x} \approx \frac{F(U_{L,i+1/2}, U_{R,i+1/2}, \gamma_i) - F(U_{L,i-1/2}, U_{R,i-1/2}, \gamma_i)}{\Delta x}.
\]

Since \( \rho h_0^m \) is frozen during the time step, the quantity \( \rho u h_0^m \) is not added to the energy flux. For radial systems the radial vector \( \mathbf{G}_r \) is unchanged for the double flux model, except the entry for the energy equation. The entry for the energy equation is \( \mathbf{G}_r(\rho E) = \rho (E - \rho h_0^m + p)v \).

The procedure to integrate the conserved variables from time level \( n \) to \( n + 1 \) for multi-stage explicit integration scheme using the double-flux model is:

1. Calculate and store \( \gamma \) and \( \rho h_0^m \) at each cell.

2. Interpolate the primitive variables (\( Y_i, p, T, u, \) and \( v \)) to the cell edges and form the double flux.

3. Update the conserved variables based on the conservation laws, the double-flux model, and the chosen time-marching method.
4. Update the primitive variables via:

\[ Y_i = \frac{\rho Y_i}{\sum \rho Y_i}, \quad u = \frac{\rho u}{\sum \rho Y_i}, \quad T = \frac{p}{\sum \rho Y_i}, \quad p = (\gamma^n - 1)\left[ \rho E - (\rho h_0^m)^n - \rho \frac{u^2 + v^2}{2} \right]. \]

(3.56)

5. Repeat steps 2-4 for each stage of the time-marching algorithm.

6. Use the primitive variables, \( \rho_i = \rho Y_i \), and momentum values calculated from the final stage as values for the next time step, \( n + 1 \), and calculate \( \gamma^{n+1} \) and \( (\rho h_0^m)^{n+1} \).

7. The total energy for time step \( n + 1 \) is given by:

\[ (\rho E)^{n+1} = \frac{\rho^{n+1}}{\gamma^{n+1} - 1} + (\rho h_0^m)^{n+1} + \rho^{n+1}(u^{n+1})^2 + (v^{n+1})^2. \]

(3.57)

The sacrifice that the double flux model makes to avoid pressure oscillations is that exact conservation is not ensured. Billet and Abgrall [77] tested this by advecting inert H\(_2\) and O\(_2\) fronts in a periodic domain where \( \gamma \) varied on 10% (one large hydrogen front) and 66% (10 smaller hydrogen fronts) of the domain. In either case the conservation errors in mass and momentum were less \( 10^{-12} \), while the conservation error in the energy was around 0.1% after 20,000 time steps for the case where \( \gamma \) varied on 10% of the domain and 1% after 60,000 time steps for the other case. While the energy conservation error may be unacceptable in certain situations, it is far less than the error introduced by pressure oscillations when the double flux model is not used. The double flux model has been successfully applied to shocked hydrogen bubble combustion [77–79].

### 3.2.6.1 Interpolation Scheme for Multi-component Gases

One problem with WENO schemes is that they can produce small, but bounded, oscillations near discontinuities. In single-component gas-dynamic flows, these small oscillations are relatively harmless. When simulating multi-component flows, small oscillations can cause the calculated mass fractions to be less than zero or greater than unity, which is unphysical. Thus, it is desirable to apply a limiter to force monotonicity near discontinuities and avoid unphysical values for mass fractions. The Monotonicity Preserving (MP) procedure of Suresh and Huynh [136] could be applied; however, this imposes a theoretical CFL restriction of
0.3. A better option is to apply the generic Total Variation Diminishing (TVD) limiter derived by Kim and Kim [137], and extend it to any interpolation method. A slope limited interpolation is defined by:

\[ Q_{i+\frac{1}{2}} = Q_i + 0.5(Q_i - Q_{i-1})\phi, \tag{3.58} \]

where \( \phi \) is the slope limiter. The TVD slope limiter used in this work is defined to be:

\[ \phi_{\text{TVD}} = \max \left[ 0, \min \left( \alpha, \alpha \frac{Q_{i+1} - Q_i}{Q_i - Q_{i-1}}, 2 \frac{\hat{Q}_{i+1/2} - Q_i}{Q_i - Q_{i-1}} \right) \right], \tag{3.59} \]

where \( \hat{Q}_{i+1/2} \) is the original interpolated variable using nonlinear error-controlled WENO with symmetric Bandwidth Optimized stencil coefficient (called WENO-SymBO in the remainder of this thesis) and \( \alpha \) is a constant that is set to 2 for this work. The multidimensional limiting process of Kim and Kim [137] could easily be applied as well. Note that applying the above TVD limiter with fifth-order LWENO reduces to the fifth-order MUSCL scheme [137].

One drawback of TVD limiters is that they clip smooth extrema. Thus, it is advantageous to apply the slope limiter only in non-smooth regions. In this work the smoothness of a variable is checked using a method adapted from Kang et al. [138]. Smooth regions are indicated by interpolating variable \( Q \) to cell center \( i \) using a centered fourth-order method and comparing it to the actual value. If error at cell \( i \),

\[ e_i = \left| -\frac{Q_{i-2,j} + 4Q_{i-1,j} + 4Q_{i+1,j} - Q_{i+2,j}}{6Q_{i,j}} - 1 \right| < \epsilon_s, \tag{3.60} \]

is small, the data are smooth and the slope limiter is not applied. In this work \( \epsilon_s \) was selected to be 0.001, which is generally recommended for most calculations. When interpolating a variable to cell face \( i+1/2 \), the error measurement is applied to cells \( i-r+2 \) through \( i+r-1 \) so that all grid points needed for the WENO scheme enter into an error measurement. The TVD limiter is applied if any one of the smoothness measurements fail. It was found that the combination of nonlinear error-controlled WENO and adaptive TVD limiters is necessary for robustness.

Even with slope limiting, some of the interpolated mass fractions occasionally become less than zero or greater than unity. In these cases it is necessary to re-normalize the mass
fractions using:

\[ Y_i = \frac{\max(\tilde{Y}_i, 0)}{\sum_{i=1}^{N} \max(\tilde{Y}_i, 0)}, \]  

(3.61)

where \( \tilde{Y}_i \) is the original interpolated mass fraction.

Godunov-based methods become very dissipative at low Mach numbers and are usually unsuitable for DNS or LES calculations of turbulent flows. Thornber et al. [139] noticed that the evaluation of inviscid fluxes using traditional Godunov-based methods (or any method that requires left- and right-interpolated states) produces a leading kinetic energy dissipation rate that is proportional to the speed of sound, which is a major source of dissipation. Recently, Thornber et al. [140] devised a simple and effective technique for reducing dissipation of Godunov-based methods with low-Mach number features. The Low-Mach (LM) adjustment blends the left and right interpolated velocities in a manner that approaches a fully centered interpolation for very low Mach number flows, but upwinds supersonic flows properly. The LM adjustment produces a kinetic energy dissipation that is not proportional to the speed of sound and is similar to Kolmogorov’s four-fifths law [141] which states that the mean dissipation rate of turbulent kinetic energy (TKE), \( \epsilon \), in the limit of large Reynolds numbers is given by \( \epsilon = -5 \left( \frac{v(x + r) - v(x) \cdot r}{r} \right)^3 / 4 \| r \| \). The LM adjustment has been found to work very well for compressible mixing problems, and produces proper decay of TKE for homogeneous decaying turbulence [140, 142].

The low-Mach number corrected interpolated velocities are defined by:

\[ \mathbf{v}_{L,LM} = \frac{\mathbf{v}_L + \mathbf{v}_R}{2} + \frac{z(\mathbf{v}_L - \mathbf{v}_R)}{2}, \]

\[ \mathbf{v}_{R,LM} = \frac{\mathbf{v}_L + \mathbf{v}_R}{2} - \frac{z(\mathbf{v}_L - \mathbf{v}_R)}{2}, \]  

(3.62)

where

\[ z = \min \left[ 1, \max \left( \frac{\sqrt{\mathbf{v}_L \cdot \mathbf{v}_L}}{c_L}, \frac{\sqrt{\mathbf{v}_R \cdot \mathbf{v}_R}}{c_R} \right) \right], \]  

(3.63)

\( \mathbf{v}_{L,R} \) are the original left- and right-interpolated velocity vectors, \( \mathbf{v}_{L,R,LM} \) are the low-Mach number adjusted interpolated velocities, and \( c \) is the speed of sound (\( c = \sqrt{\gamma p/\rho} \)). This simple correction has been shown to work very well for compressible turbulent flows [86, 140, 142] and produces a proper dissipation of TKE for homogeneous decaying turbulence.
It would also be advantageous to apply the following adjustment to all of the primitive variables in smoothly varying regions to reduce numerical dissipation of contact surfaces even further [140]. Care must be taken, since applying the LM adjustment procedure on slowly moving material interfaces will result in increased dissipation of the density, mass fractions, and temperature. The technique developed by Kim and Kim [124] centers the interpolated variable only in smoothly varying regions and leaves the original interpolation alone if the variation is too rapid. The useful concept of Kim and Kim [124] is slightly modified to produce a LM adjustment scheme suitable for scalars:

\[ Q_{L,LM} = Q_L + \frac{\max[0, (Q_R - Q_L)(Q_{L,SB} - Q_L)]}{(Q_R - Q_L) |Q_{L,SB} - Q_L|} \min\left[ (1 - z) \frac{|Q_R - Q_L|}{2}, |Q_{L,SB} - Q_L| \right], \]
\[ Q_{R,LM} = Q_R + \frac{\max[0, (Q_L - Q_R)(Q_{R,SB} - Q_R)]}{(Q_L - Q_R) |Q_{R,SB} - Q_R|} \min\left[ (1 - z) \frac{|Q_R - Q_L|}{2}, |Q_{R,SB} - Q_R| \right], \]

(3.64)

where \( Q_{SB} \) is the edge interpolation of variable \( Q \) using Eq. (3.58) with superbee slope limiter, \( \phi_{SB} \). The superbee slope limiter is:

\[ \phi_{SB} = \max\left[ 0, \min\left( 2\alpha \frac{Q_{i+1} - Q_i}{Q_i - Q_{i-1}}, 1 \right), \min\left( \frac{Q_{i+1} - Q_i}{Q_i - Q_{i-1}}, \alpha \right) \right], \]

(3.65)

where \( \alpha = 2 \). Equation (3.64) is used to adjust \( T, p, \) and \( Y_i \). However, Eq. (3.62) is used to adjust the velocity vector regardless if the velocity vector is smoothly or rapidly varying.

### 3.2.6.2 Choice of Interpolation Variable for Multi-component Gases

It is well known that the choice of which set of variables (primitive, conservative, characteristic, etc.) to interpolate has a drastic effect on the quality of the solution. Interpolating the primitive variables, \( P = (Y_i, u, v, p, T)^T \), directly is computationally efficient but is very prone to producing oscillations near shock waves, as shown in Figure 3.5a. Interpolating characteristic variables, although computationally expensive, is generally preferred to avoid oscillations near shocks when using higher-order methods [143].

Since the specific heat ratio is not constant and the double-flux model is used, the procedure for locally transforming to and from characteristic variables is more involved than it is for constant property calculations. First, the specific heat ratio and primitive variables are estimated at the cell edge using the arithmetic average, \( \gamma_{i+1/2} = 0.5(\gamma_i + \gamma_{i+1}) \)
and $P_{i+1/2} = 0.5(P_i + P_{i+1})$. The primitive variables are converted to faux conservative variables, $U'$, using definition of the conservative variables and Eq. (3.54) with $\gamma = \gamma_{i+1/2}$ and $h_0^m = 0$ at all grid points in the interpolation stencil:

$$U'_j = f(P_j, \gamma_{i+1/2}, h_0^m = 0); \quad j = i - r + 1, \cdots, i + r,$$

(3.66)

where $f$ represents the set of functions that transform the primitive variables to conservative for the double-flux model. The faux conservative variables are then converted to characteristic variables, $C$ using:

$$C_j = L_{i+1/2} \cdot U'_j; \quad j = i - r + 1, \cdots, i + r,$$

(3.67)

where $L_{i+1/2}$ is the array of left eigenvectors of the flux Jacobian, (given by Eq. 3.70) calculated using $P_{i+1/2}$ and $\gamma_{i+1/2}$. Next the characteristic variables are interpolated to the cell edge using the slope limited nonlinear error controlled WENO-SymBO. The interpolated characteristic variables, $C_{i+1/2}^L$ and $C_{i+1/2}^R$, are converted back to primitive variables:

$$P_{i+1/2}^L = f'(R_{i+1/2}^L \cdot C_{i+1/2}^L, \gamma_{i+1/2}, h_0^m = 0),$$

$$P_{i+1/2}^R = f'(R_{i+1/2}^R \cdot C_{i+1/2}^R, \gamma_{i+1/2}, h_0^m = 0),$$

(3.68)

where $R_{i+1/2}$ is the array of right eigenvectors (given by Eq. 3.69) and $f'$ represents the set of functions that map $U'$ to $P$ for the double-flux model. The LM-adjustment procedure is then applied to the interpolated primitive variables for producing the final interpolation.

There are a variety of other methods for locally transforming to characteristic variables such as using $\gamma_i$ and $P_i$ to linearize the left stencil and $\gamma_{i+1}$ and $P_{i+1}$ or using a Roe-averaged state at the interface [143]. It was found that simple arithmetic averaging is sufficient in this work. For the double flux model, the matrix of right eigenvectors for the x-flux vector, $R$ is
Figure 3.5: Comparison of variable interpolation method for (a) colliding shock problem with $u_L = -u_R = 100 \, \text{m/s}$, $p = 1 \, \text{atm}$, and $T = 1000 \, \text{K}$ and (b) hydrogen bubble advection.

given by:

$$
\mathbf{R} = \begin{bmatrix}
Y_1 & 1 & 0 & \cdots & 0 & 0 & Y_1 \\
Y_2 & 0 & 1 & \cdots & 0 & 0 & Y_2 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
Y_{N_9} & 0 & \cdots & 1 & 0 & Y_{N_9} \\
u - c & u & \cdots & u & 0 & u + c \\
v & v & \cdots & v & 1 & v \\
H - uc & \frac{\|v\|^2}{2} & \cdots & \frac{\|v\|^2}{2} & v & H + uc
\end{bmatrix}
$$

and the matrix of left eigenvectors, $\mathbf{L}$, is given by:

$$
\mathbf{L} = \frac{1}{c^2} \begin{bmatrix}
\phi + uc & \cdots & \phi + uc & -\frac{\gamma u + c}{2} & -\frac{\gamma}{2} v & \frac{\gamma}{2} \\
c^2 - Y_1 \phi & -Y_1 \phi & \cdots & -Y_1 \phi & Y_1 \gamma u & Y_1 \gamma v & -Y_1 \gamma \\
-Y_2 \phi & c^2 - Y_2 \phi & \cdots & -Y_2 \phi & Y_2 \gamma u & Y_2 \gamma v & -Y_2 \gamma \\
\vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
-Y_{N_9} \phi & \cdots & -Y_{N_9} \phi & c^2 - Y_{N_9} \phi & Y_{N_9} \gamma u & Y_{N_9} \gamma v & -Y_{N_9} \gamma \\
-vc^2 & \cdots & -vc^2 & -vc^2 & 0 & c^2 & 0 \\
\phi - uc & \cdots & \phi - uc & -\frac{\gamma u - c}{2} & -\frac{\gamma}{2} v & \frac{\gamma}{2}
\end{bmatrix}
$$
where $\hat{\gamma} = \gamma - 1$, $\phi = \hat{\gamma}|\mathbf{v}|^2/2$, and $H = E + p/\rho$. The eigenvectors for the y-flux vector can be computed by rotating the coordinate system to x-direction.

One issue that surfaced when interpolating characteristic variables is that small temperature spikes, shown in Figure 3.5b, form when advecting sharp material interfaces. These temperature spikes near the material interface are unphysical. While these temperature spikes are normally quite small and can be tolerated in many situations, they can falsely initiate chemical reactions. Interpolating primitive variables does not produce temperature spikes at the cost of slightly increased numerical diffusion (shown by the dashed lines in Figure 3.5b). A hybrid scheme that interpolates characteristic variables near shock waves and primitive variables elsewhere was designed to take advantage of both methods. The characteristic variable are interpolated method if the error in pressure, $e^p$,

$$e^p = \max(e^p_{x,ij}, e^p_{y,ij}) < \epsilon_s; \quad l = i - r + 1, \ldots, i + r,$$

(3.71)

and

$$\max(p_{lj}) - \min(p_{lj}) < \Delta p_s; \quad l = i - r + 1, \ldots, i + r.$$

(3.72)

$\Delta p_s$ is a parameter that must be set based on the magnitude of the pressure jump of shock waves in a particular problem. The errors $e^p_{x,ij}$ and $e^p_{y,ij}$ are the smoothness measurements of pressure in the x- and y-directions, respectively, at cell $ij$ using Eq.(3.60). The slope limiter is applied to all characteristic fields, otherwise the oscillations that form near shock waves become more pronounced. Dissipation introduced by the slope limiter is sufficient to suppress the small temperature spikes when a shock wave interacts with a material interface.

The application of the hybrid scheme on the colliding shock problem is shown in Figure 3.5a. Applying the hybrid scheme with a high $\Delta p_s$ that is near the pressure jump across the shock wave provides little improvement over interpolating the primitive variable, while choosing a small $\Delta p_s$ give results that are nearly identical to those obtained from interpolating characteristic variables. Since the pressure is constant for the H$_2$ bubble advection problem shown in Figure 3.5b, the characteristic variables are never interpolated and the hybrid scheme reduces to the primitive variable interpolation scheme.

Perhaps a simpler approach to reduce spurious oscillations near shocks would be to switch to a more dissipative method, such as MUSCL with the minmod slope limiter, near shocks. However, this approach was found to be significantly more dissipative than the characteristic-based approach, especially when shock waves interact with material interfaces.
An extensive series of verification tests for the gas-phase solver are given in Appendix C. More complex calculations that serve as validation purposes for the reacting gas-dynamics solver are detailed in Chapter 5.

3.2.7 Liquid Phase Interpolation Method and Flux Evaluation Scheme

In this work the compressible droplet is modeled using a barotropic [i.e., $p = p(\rho)$] one-fluid model for a cavitating liquid. Thus, the governing equations for the liquid region are the compressible Navier-Stokes equations, Eq. (3.1), with:

$$
U = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho e
\end{bmatrix}, \quad 
F = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho u v \\
\rho e u
\end{bmatrix}, \quad 
G = \begin{bmatrix}
\rho v \\
\rho u v \\
\rho v^2 + p \\
\rho v e
\end{bmatrix}, \quad 
F_v = \begin{bmatrix}
0 \\
\sigma_{xx} \\
\sigma_{xy} \\
-q_x
\end{bmatrix}, \quad 
G_v = \begin{bmatrix}
0 \\
\sigma_{yx} \\
\sigma_{yy} \\
-q_y
\end{bmatrix}.
$$

(3.73)

The numerical fluxes for the barotropic equation of state are evaluated using a hybrid method. Characteristic-based LLF flux with nonlinear error-controlled TVD slope limited WENO-SymBO is used if the pressure is greater than the saturation pressure. If the liquid mixture is cavitating, MUSCL with the minmod slope limiter is used to interpolate the primitive variables in conjunction with with the dissipative Rusanov flux. The eigenvector arrays for the x-flux vector for a generic barotropic fluid in two dimensions are:

$$
R = \begin{bmatrix}
1 & 0 & 0 & 1 \\
\frac{u-c}{2c} & 0 & 0 & \frac{u+c}{2c} \\
u & 1 & 0 & u \\
e & 0 & 1 & e
\end{bmatrix}, \quad 
\text{and} \quad 
L = \begin{bmatrix}
\frac{u+c}{2c} & -\frac{1}{2c} & 0 & 0 \\
-u & 0 & 1 & 0 \\
-e & 0 & 0 & 1 \\
-\frac{u-c}{2c} & \frac{1}{2c} & 0 & 0
\end{bmatrix}.
$$

(3.74)

Verification tests for the liquid solver are given in Appendix C. The hybrid flux evaluation scheme works well for water when the CFL number is 0.5 and directionally unsplit; however, liquid Al is a much stiffer fluid and it was found that using the directionally unsplit hybrid flux evaluation scheme produced severe even-odd oscillations as shown in Figure 3.6. Using the higher dissipation minmod slope limited MUSCL approach with the Rusanov flux integrated in a directionally-split manner suppressed these oscillations.
Figure 3.6: Effect of directional splitting and liquid flux evaluation method on the even-odd instability on a cylindrical gas-liquid Riemann with pressurized aluminum.

3.2.8 Riemann Solver for the Dusty Phase

The flux evaluation methods given above only apply to the continuous phase, the following simplified Riemann solver for the dispersed condensed phase products [144]:

\[
F_c = \begin{cases} 
F_c(U_{L,c}) & \text{if } u_{c,L} \geq 0 \text{ and } u_{c,R} > 0 \\
F_c(U_{R,c}) & \text{if } u_{c,L} < 0 \text{ and } u_{c,R} \leq 0 \\
F_c(U_{L,c}) + F_c(U_{R,c}) & \text{if } u_{c,L} > 0 \text{ and } u_{c,R} < 0 \\
0 & \text{if } u_{c,L} < 0 \text{ and } u_{c,R} > 0,
\end{cases}
\] (3.75)

where \( U_c = (\alpha_c \rho_c, \alpha_c \rho_c u_c, \alpha_c \rho_c v_c, \alpha_c \rho_c E_c, N_c)^T \). The dusty gas equations are hyperbolically degenerate (i.e., all of the eigenvalues are real, but not all of the eigenvectors are linearly independent), which can be somewhat unstable to integrate if using high-order Godunov-based methods. Thus, the MUSCL approach utilizing minmod slope limiter was applied to the condensed phase primitive variables rather than the low-dissipation schemes used for the gas-phase region.
3.2.9 Thermodynamic Property Evaluation

Expressions for evaluating the thermodynamic properties are given in Appendix A. Calculating each of these thermal properties as needed using NASA polynomials would be quite expensive. Thus, the specific heat, enthalpy, and entropy are stored in linear interpolation tables which are formed at the start of the calculation. Once the temperature interval is known, any pure species thermodynamic property can be calculated with a single multiply and add. Unless otherwise noted the temperature increment in the property tables is $\Delta T = 1$ K.

3.3 Integration of the Parabolic Step

3.3.1 Calculation of the Diffusion Fluxes and Viscous Stresses

The diffusion fluxes are calculated conservatively using standard second-order methods where the gradients normal to a cell face are given by:

$$
\frac{dQ}{dx} \bigg|_{i+1/2} \approx \frac{Q_{i+1} - Q_i}{\Delta x},
$$

(3.76)

and gradients tangential to a cell face are approximated using:

$$
\frac{dQ}{dy} \bigg|_{i+1/2,j} \approx \frac{Q_{i+1,j+1} + Q_{i,j+1} - Q_{i+1,j-1} - Q_{i,j-1}}{4\Delta y}.
$$

(3.77)

3.3.2 Integration of the Parabolic Operator

The parabolic term is integrated in time using the second-order explicit Runge-Kutta-Chebyshev (RKC) [145] scheme, which has extended stability bounds through the use of an arbitrary number of stages. The scheme to integrate the parabolic terms,

$$
\frac{dU}{dt} = \frac{\partial F_v}{\partial x} + \frac{\partial G_v}{\partial y} = P_{xy},
$$

(3.78)
from time level \( n \) to \( n + 1 \) using the fully explicit RKC scheme with \( m \) stages goes as follows:

\[
\begin{align*}
U_0 &= U^n \\
F_0 &= P_{xy}(U_0) \\
U_1 &= U_0 + \tilde{\mu}_1 \Delta t F_0 \\
\text{Loop: } j &= 2, m \\
F_{j-1} &= P_{xy}(Q_{j-1}) \\
U_{j} &= (1 - \mu_j - \nu_j) U_0 + \mu_j U_{j-1} + \nu_j U_{j-2} + \tilde{\mu}_j \Delta t F_{j-1} + \tilde{\gamma}_j \Delta t F_0 \\
\text{End Loop}
\end{align*}
\]

\[
U^{n+1} = U_m,
\]

where the coefficients are given by:

\[
\tilde{\mu}_1 = b_1 \omega_1, \quad \tilde{\mu}_j = \frac{2b_j \omega_1}{b_{j-1}}, \quad \mu_j = \frac{2b_j \omega_0}{b_{j-1}}, \quad \nu_j = -\frac{b_j}{b_{j-2}}, \quad \tilde{\gamma}_j = -a_{j-1} \tilde{\mu}_j
\]

for \( j = 2, \cdots, m \). The parameters \( a, b, \) and \( \omega \) are given by

\[
\begin{align*}
\omega_0 &= 1 + \frac{\epsilon}{m^2}, \quad \omega_1 = \frac{T_m'(\omega_0)}{T_m''(\omega_0)}, \quad b_0 = b_2, \quad b_1 = \frac{1}{\omega_0}, \\
b_j &= \frac{T_j''(\omega_0)}{(T_j'(\omega_0))^2}, \quad a_j = 1 - b_j T_j(\omega_0),
\end{align*}
\]

where \( \epsilon = 10 \). \( T_j(x) \) are Chebyshev polynomials of the first kind:

\[
T_0(x) = 1, \quad T_1(x) = x, \quad T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x).
\]

The number of stages, \( m \), is determined using the criterion:

\[
\Delta t \sigma(P'_{xy}(Q,t)) \leq \beta(m),
\]

where \( \sigma(P'_{xy}) \) is the spectral radius of the Jacobian of \( P_{xy} \), and \( \beta(m) \) is the stability boundary [145],

\[
\beta(m) = \begin{cases} 
2, & m \leq 2 \\
(m^2 - 1) \{0.340 + 0.189[2/(m - 1)]^{1.3}\}, & m > 2.
\end{cases}
\]
The spectral radius scales as $(\Delta x)^{-2}$ for the diffusion equation and the time step scales with $\Delta x$. Thus, $\Delta t \sigma(P'_{xy})$ scales with $(\Delta x)^{-1}$. Since $\beta(m)$ roughly scales with $m^2$, the number of RKC stages (hence the parabolic integration work) scales with $(\Delta x)^{-1/2}$. RKC significantly reduces computational effort in comparison to sub-cycling Euler’s method or RK2 many times and produces a practical method for explicitly marching parabolic systems on fine meshes where the time-step size would otherwise be dominated by the parabolic terms. The RKC scheme was found to give results that are nearly identical to sub-cycling for the numerical experiments presented in Sections 8 and 9 at significantly reduced computational expense for many cases. Since RKC reduces to second-order Runge-Kutta when $m = 2$, there is relatively little extra computational cost when using RKC on larger meshes and the additional stages are not necessary for stabilization.

In this work, the spectral radius is approximated as:

$$\sigma(P'_{xy}) \approx \chi \max \left[ 8 \frac{\lambda}{\rho C} \Delta^2, 8 \frac{D_{l,mix}}{\Delta^2}, 1 \frac{29 \mu}{3 \rho} + \frac{5 \kappa}{\rho} \right],$$

(3.85)

where $\Delta = \min(\Delta x, \Delta y)$. Accounting for all nonlinearities when calculating the spectral radius, such as temperature- and species-dependent properties, would be inefficient due to the complex expressions that arise. In place of exact analytical expressions, the linear spectral radius is simply multiplied by a parameter, $\chi$, which is set to 1.5 unless otherwise noted.

An example of the application of the RKC scheme to solving the problem:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2},$$

$$T(0, x) = \begin{cases} 100 & \text{if } |x| < 1 \\ 0 & \text{if } |x| \geq 1, \end{cases}$$

(3.86)

which has the exact solution [146]:

$$T(t, x) = 50 \left[ \operatorname{erf} \left( \frac{x + 1}{2 \sqrt{t}} \right) - \operatorname{erf} \left( \frac{x - 1}{2 \sqrt{t}} \right) \right],$$

(3.87)

shown in Figure 3.7. The solution was advanced using RKC and a grid with 2000 cells. The time step restriction using standard explicit methods is $12.5 \mu s$ where RKC is stable for all the time steps used. Using a single time step of 0.005 s would require 400 Euler steps, while RKC only required 47 stages. Just as with implicit methods, even though a method is stable...
Figure 3.7: Comparison of the exact solution to the RKC solution of Eq. (3.86) at times of 0.005 s, 0.05 s, and 0.5 s.

for any time-step size that does not mean very large time-step sizes should be used. RKC produced a stable result at a single time step of 0.5 s, but with substantial error.

3.3.3 Transport Property Evaluation

Detailed expressions for evaluating the transport properties for both ideal gases and the liquids are given in Appendix A. Evaluating each transport property directly from kinetic theory would be computationally expensive and inefficient. To increase computational efficiency, all transport properties are evaluated using linear interpolation tables that are formed at the start of each calculation.

3.4 Integration of the Source Term Vector

Integration of the source terms in the governing equations requires the solution of the local system of ODEs:

\[
\frac{dU}{dt} = S,
\]

where \( S \) is the source term vector arising from chemical reactions, phase change, particle drag, etc. The evaluation of the source term vector is given in detail in Chapter 2 and Appendix A. In general, the source term forms a stiff system of ODEs due to chemical
reactions. A system of ODEs is considered to be stiff if there is great discrepancy between
the maximum and minimum real part of the source term Jacobian eigenvalues. In this work
either the ODE solver DVODE_F90 [147], which is a Fortran 90 version of DVODE [148], or
CHEMEQ2 [149] are used.

When used to integrate stiff ODEs, VODE_F90 uses a variable-order backwards differ-
entiation formula (BDF) to implicitly integrate the system of the ODEs. A generic BDF
method of order \( m \) is:

\[
Q^{n+1} = \sum_{i=1}^{m} \alpha_i y_{n+1-i} + \Delta t \beta_0 \dot{Q}^{n+1},
\]

where \( \alpha_i \) are constants that depend on the order \( m \) and \( \beta_0 = 1/\sum_{i=1}^{m} i^{-1} \). For example the
second-order BDF method is:

\[
Q^{n+1} = \frac{4}{3} Q^n - \frac{1}{3} Q^{n-1} + \frac{2}{3} \Delta t \dot{Q}^{n+1}.
\]

Since analytical evaluation of the source term Jacobian necessary to solve the nonlinear
system of equations for the BDF can be complicated, the source-term Jacobian is obtained
numerically using finite differences. The resulting nonlinear system of equations are solved
using Newton-Raphson method with a dense, direct linear equation solver.

The relative and absolute error tolerances of the species densities are set to \( 10^{-9} \) and
\( 10^{-15} \) for DVODE, respectively. Unless otherwise noted, the error tolerance for CHEMEQ2
was set to \( 10^{-8} \) with four corrector stages.

Numerical libraries such as Cantera [150] already exist for integrating gas-phase chemical
kinetic source terms; however, the source terms for a multiphase reacting flow are more
general and have additional terms that are not present in single-phase reacting flow. Thus,
a custom library based on VODE_F90 was written to integrate the source terms.

In many cases the integration of the chemical reaction source term can dominate the
execution time. To expedite the evaluation of the reaction rates, the forward and backward
chemical kinetic rate constants are stored in linear interpolation tables of the form \( k_{f,b} =
\]

\[
a_i T + b_i,
\]

similar to the specific heats for the double flux model. In many circumstances there
are regions of the calculation where the solution is essentially constant. It would be wasteful
to call the chemistry solver in cells where the variable vectors are nearly identical. In this
model the chemistry solver is only called if the mass fractions vary by more than \( 10^{-10} \),
the temperature varies by more than 0.1 K, or the pressure varies by more than 0.001 Pa,
otherwise the solution from the previous call to the chemistry integration routine is used. This practice decreased the total execution time by about half for the 1-D laminar premixed flame propagation problem, without affecting the overall solution.

In this thesis global time-step size is based on the hydrodynamic CFL limit, regardless of how stiff the source term vector is. For most compressible chemically reacting flow simulations, the time-step size is usually small. Thus, selecting the global time-step size based on the CFL condition is not expected to introduce significant error in most cases with the present numerical method. It was found that there was little difference between calculations that limited the global time-step size based on the CFL criterion and calculations where the time steps were fixed at a very small number (see Figure 5.12).

3.5 Numerical Boundary Conditions

Boundary conditions for multi-dimensional compressible flow can be tricky [151]. If naïve extrapolation methods are used, unphysical pressure waves can propagate from the boundary to the interior of the domain. In some cases these unphysical waves can degrade the quality of the solution. There have been several methods developed to suppress these waves [151]. In this work the Navier-Stokes Characteristics Boundary Conditions (NSCBC) of Poinsot and Veynante [152] was used. The extent of the domain will be chosen such that the liquid phase region should never leave the domain; thus the extensions of NSCBC to real gases [153] does not need to be considered in this work.

The fundamental idea of NSCBC is to first cast the governing equations into a Local One Dimensional Inviscid (LODI) form normal to the boundary. The LODI relations, definitions of wave strengths, and physical boundary conditions are used to eliminate the strength of incoming rogue waves. Rather than integrating the conservation laws directly, the outgoing wave strengths are used to evaluate the numerical flux gradients normal to the boundary. If a boundary with its normal in the positive x-direction is considered, the characteristic wave strengths, \( L_i \), can be computed as follows:

\[
L_1 = (u - c) \left( \frac{\partial p}{\partial x} - \rho c \frac{\partial u}{\partial x} \right) \quad \text{for} \quad \lambda_1 = u - c, \tag{3.91}
\]

\[
L_2 = u \left( c^2 \frac{\partial \rho}{\partial x} - \frac{\partial p}{\partial x} \right) \quad \text{for} \quad \lambda_2 = u, \tag{3.92}
\]

\[
L_3 = u \frac{\partial v}{\partial x} \quad \text{for} \quad \lambda_3 = u, \tag{3.93}
\]
\[ \mathcal{L}_4 = u \frac{\partial w}{\partial x} \quad \text{for} \quad \lambda_4 = u, \]  
(3.94)

\[ \mathcal{L}_5 = (u + c) \left( \frac{\partial p}{\partial x} + \rho c \frac{\partial u}{\partial x} \right) \quad \text{for} \quad \lambda_5 = u + c, \]  
(3.95)

\[ \mathcal{L}_{5+k} = u \frac{\partial Y_k}{\partial x} \quad \text{for} \quad \lambda_{5+j} = u; \quad j = 1, \cdots, N_g. \]  
(3.96)

The above definitions can only be used to calculate the amplitude of waves leaving the domain. The LODI relations are used to connect incoming and outgoing wave amplitudes in conjunction with the physical boundary conditions. In terms of the primitive variables, the LODI relations are:

\[ \frac{\partial \rho}{\partial t} + \frac{1}{c^2} \left[ \frac{\mathcal{L}_5 + \mathcal{L}_1}{2} + \mathcal{L}_2 \right] = 0, \]  
(3.97)

\[ \frac{\partial u}{\partial t} + \frac{\mathcal{L}_5 - \mathcal{L}_1}{2\rho c} = 0, \]  
(3.98)

\[ \frac{\partial v}{\partial t} + \mathcal{L}_3 = 0, \]  
(3.99)

\[ \frac{\partial w}{\partial t} + \mathcal{L}_4 = 0, \]  
(3.100)

\[ \frac{\partial p}{\partial t} + \frac{\mathcal{L}_5 + \mathcal{L}_1}{2} = 0, \]  
(3.101)

\[ \frac{\partial Y_k}{\partial t} + \mathcal{L}_{k+5} = 0; \quad k = 1, \cdots, N_g \]  
(3.102)

\[ \frac{\partial T}{\partial t} + \frac{T}{\gamma \rho} \left[ -\mathcal{L}_2 + \frac{1}{2}(\gamma - 1)(\mathcal{L}_5 + \mathcal{L}_1) \right] = 0. \]  
(3.103)

Once all of the incoming and outgoing wave strengths are determined, the conservation laws on the boundary are updated via

\[ \frac{\partial \rho}{\partial t} + d_1 + \frac{\partial \rho v}{\partial y} = 0, \]  
(3.104)

\[ \frac{\partial \rho u}{\partial t} + ud_1 + \rho d_3 + \frac{\partial \rho uv}{\partial y} = 0, \]  
(3.105)

\[ \frac{\partial \rho v}{\partial t} + vd_1 + \rho d_4 + \frac{\partial \rho vv}{\partial y} + \frac{\partial p}{\partial y} = 0, \]  
(3.106)

\[ \frac{\partial \rho Y_k}{\partial t} + Y_k d_1 + \rho d_{k+5} + \frac{\partial \rho Y_{kv}}{\partial y} = 0, \]  
(3.107)
\[
\frac{\partial \rho E}{\partial t} + \frac{u^2 + v^2}{2} d_1 + \frac{d_2}{\gamma - 1} + \rho u d_3 + \rho v d_4 + \frac{\partial v (\rho E + p)}{\partial y} = 0,
\]
(3.108)

where
\[
\begin{align*}
    d_1 &= \frac{1}{c^2} \left[ \frac{L_5 + L_1}{2} + L_2 \right], \\
    d_2 &= \frac{L_5 + L_1}{2}, \\
    d_3 &= \frac{L_5 - L_1}{2\rho c}, \\
    d_4 &= L_3, \\
    d_5 &= L_4, \\
    d_{k+5} &= L_{k+5}; k = 1, \cdots, N_g.
\end{align*}
\]

The above equations are written for boundary conditions in the x-direction; NSCBC boundary conditions for the other directions are similar, with the exception that the coordinate system needs to be rotated.

The LODI relations provide conditions on the hyperbolic portion of the Navier-Stokes equations, but not the parabolic portion. Poinsot and Veynante [152] recommend using a simple zero-curvature (i.e., zero diffusion flux gradient) condition to estimate the viscous and diffusion fluxes at inlets and outlets.

The general procedure for using the NSCBC is to first pick physical boundary conditions and then use the LODI relations to relate the strengths of the incoming waves to the outgoing waves. The strength of the outgoing waves is simply determined by finite differencing of the interior data. After all of the wave strengths have been determined, the vector \(d\) is calculated. Finally Eqs. (3.104) through (3.108) are used to advance the conserved variables at the boundary.

### 3.5.1 Non-Reflecting Inlets

Based on wave speeds, all waves enter the domain, except for one if the inlet is subsonic. Depending on which side of the domain the inlet is located, either \(L_1\) (left side) or \(L_5\) (right side) will be the outgoing wave. To ensure that no spurious waves enter the domain, all the incoming wave strengths are set to zero. The strength of the outgoing wave, say \(L_1\), is calculated using standard finite differences of interior data points.
Note that when a non-reflection BC is enforced, none of the primitive variables are enforced at the boundary. If conserved variables are not allowed to wander the inlet will not be totally non-reflecting. When the inlet is supersonic, all of the waves are incoming and all of the conserved variables can be imposed directly.

3.5.2 Non-Reflecting Outlets

In the subsonic case there is only one incoming wave, $L_1$ if the outlet is on the right side of the domain, which is set to zero strength. All of the other waves strengths are calculated using forward differencing of the interior grid points. If the outlet is supersonic, all waves are outgoing and are calculated using interior data.

3.5.3 Slip Wall

Even though the slip walls are not directly used in this work, symmetry BCs can be viewed as a slip wall with zero diffusive fluxes. In this case the only physical boundary condition that can be specified is $u = 0$. Using the LODI relation for the normal velocity gives:

$$L_5 = L_1. \quad (3.115)$$

Since $u = 0$, $L_2, L_3, L_4, L_6, \ldots, L_{5+N_x}$ are all zero. The only outgoing wave is $L_1$ if the wall is on the left side of the domain and $L_5$ if the wall is on the right side of the domain. As with the other BCs, the strength of the outgoing wave is calculated using finite differences of the interior data. Equation (3.115) is used to set the strength of the incoming wave. Finally, Eqs. (3.104) through (3.108) with the exception of the normal momentum equation Eq. (3.105) are advanced in time. The gradients of diffusion fluxes are set to zero.

3.6 Adaptive Mesh Refinement

To reduce computational expense, adaptive mesh refinement (AMR) was used to place the finest cells only where they are needed. Since the high-order edge interpolation methods require a uniform grid, many common AMR algorithms cannot be used. In this work the block structured AMR (SAMR) technique first introduced by Beger and Oliger [154] and later extended by Berger and Collela [155] is used. Rather than using one mesh with different
grid spacings, the SAMR method uses many blocks (or sub-grids) with different, but uniform grid spacing.

### 3.6.1 Structured Adaptive Mesh Refinement Methodology

As stated above, SAMR uses multiply nested uniform grids at different refinement levels as shown in Figure 3.8. The finest grids are contained entirely in the subset of the grids that are one level coarser than it; $\Omega_{\text{ref, max}} \subset \Omega_{\text{ref, max}-1} \subset \Omega_{\text{ref, max}-2} \subset \cdots \subset \Omega_1$, where $\Omega_i$ is the sub-domain with refinement level $i$ and $\Omega_1$ is the overall computational domain with no refinement. The boundary conditions of an interior sub-grid are obtained by filling guard cells that surround it. The guard cells are populated either by direct copying if the neighbor block is at the same level of refinement or by interpolation if it is not. Restriction and prolongation are two of the most important data movement operations needed to propagate data from coarse grids to fine grids and vice versa, fill guard cells, and initialize data on newly refined sub-grids.
3.6.1.1 Restriction

Restriction is the action of moving data from a fine child block to its coarser parent block. The most common restriction method is conservative restriction introduced by Berger and Collela [155]. The conservative restriction method simply averages the data on the finer child cells and passes that value to the coarser parent cell. This is the only restriction method that is guaranteed to be conservative; other interpolation methods are available, but may lead to conservation errors.

Special care must be taken when combining the level set method with SAMR during the restriction process. Consider the following example where the refinement ratio between grid levels is two and a liquid/gas flow with densities of 1000 and 1 kg/m$^3$, respectively, is being calculated. If three of the cells are in the liquid phase and the other is in the gas, applying the conservative restriction algorithm would give a density of 750 kg/m$^3$ in the parent cell, which is unphysical; far too low to be a liquid and far too high to be a gas.

Nourgaliev et al. [44] came up with a solution to this problem. First they restrict the level set function to the coarser grid. The fluid variables in the parent cell are restricted by interpolating variables from the fluid signed with the parent cell using a method suitable for scattered data sets such as natural neighbor interpolation or Shepard’s interpolation [156–158]. For example, if the parent cell is liquid only child cells containing liquid are used in the restriction process. The restriction problem is avoided entirely in this work by forcing grid to be at the finest level if it is closer than six cells to the interface.

3.6.1.2 Prolongation

Prolongation is the opposite operation of restriction; it is process of moving data from a coarse grid to a finer grid. In most applications, prolongation is performed using linear interpolation or zeroth-order direct injection from the parent cell, which are both conservative. Higher-order interpolation can be used if data is smooth and conservation is not a concern.

Similar to restriction, standard prolongation schemes can lead to unphysical values when the level set method is used.

3.6.1.3 Conservative Edge Fluxes

One of the disadvantages of SAMR is that edge fluxes on the border of a sub-grid need to be formed twice, once for each neighbor sharing the edge. If the neighbors are on the
same refinement level, data used to form the flux is identical on both blocks. Thus, the flux will be calculated identically for each sub-grid. If the neighbors are on different refinement levels, the edge flux may differ due to the restriction and prolongation processes used to fill guard cells. The lack of conservation at boundaries between fine and coarse blocks that this introduces may destroy the quality of the solution. Berger and Collela [155] came up with a solution to this problem by using the average of the fine edge fluxes to advance the solution on the coarser sub-grid. For example the flux gradient for a cell with a fine neighbor to the right is:

\[
\frac{\partial F}{\partial x} = \frac{1}{\Delta x_{\text{coarse}}} \left[ \frac{1}{r} \left( \sum_{k=1}^{r} F_{i+1/2,k,\text{fine}} \right) - F_{i+1/2,j,\text{coarse}} \right],
\]

(3.116)

where \( r \) is the refinement ratio between the grid levels. The solution on the fine cells is left unchanged.

The conservative coarse/fine flux evaluation procedure does not have to be modified to make it suitable for cells cut by the liquid/gas interface since the interface between gas and liquid regions is contained entirely on the finest grid level.

It was found that in this work that the formal conservative edge flux treatment was not needed if the grid is refined well in advance of any discontinuities or steep gradient in the flow-field. Abandoning the strict conservative edge flux treatment also avoids several synchronization points, decreasing communication costs between processors.

### 3.6.2 Refinement Criterion

In the original SAMR methods [155], refinement tagging was performed by calculating a time step twice; the first one at the full time step, \( \Delta t \), and the second by two steps of \( 1/2 \Delta t \). Richardson extrapolation was used to estimate the error between the two solutions. If the error on a block is too high, it is marked for refinement. Conversely, if the error on a block is sufficiently low it is marked for coarsening (or derefinement). This method is expensive and will not be used.

Nourgaliev et al. [44] use the following simpler scheme to mark a grid for refinement. First they calculate

\[
\Delta_0 \psi = \max(|\psi_{i,j} - \psi_{i-1,j}|, |\psi_{i,j} - \psi_{i+1,j}|),
\]

\[
\Delta_1 \psi = \psi_{i+1,j} - \psi_{i-1,j},
\]

\[
\Delta_2 \psi = \psi_{i+2,j} - \psi_{i-2,j},
\]

(3.117)
in every direction (x, y, and both diagonal directions), where \( \psi \) is a variable used for refinement tagging (either \( p \) or \( \rho \)). The cell is tagged for refinement if any one of the following is satisfied:

\[
\alpha |\Delta_2 \psi| \leq |\Delta_1 \psi|, \\
\Delta_1 \psi \Delta_2 \psi < 0, \\
\Delta_0 \psi > \epsilon \Delta x.
\]  

\( (3.118) \)

In this method, there are two free parameters to choose, \( \alpha \) and \( \epsilon \). A value of \( \alpha = 0.9 \) is usually sufficient. The gradient tolerance parameter, \( \epsilon \), needs to be tuned for each calculation.

The refinement criterion of Sun and Takayama [159] is applied to this work. A parameter \( \phi \) is calculated in all four directions (x, y, and both diagonals):

\[
\phi = \frac{|\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}|}{\alpha_{\text{Sun}}|\psi_{i,j}| + |\psi_{i+1,j} - \psi_{i-1,j}|},
\]  

\( (3.119) \)

where \( \alpha_{\text{Sun}} = 0.03 \). The calculation of \( \phi \) is similar for the other directions. Defining \( E_{ij} = \max(\phi_i, \phi_j, \phi_{ij}, \phi_{ji}) \) and \( E_{\max} = \max(E_{ij}) \), the grid is marked for refinement if \( E_{\max} > 0.03 \) and marked for derefinement if \( E_{\max} < 0.01 \).

A criterion that has good performance in steep but smooth regions is the error measurement used by the FLASH astrophysics group [160], whose error measurement is defined as:

\[
E_{ij} = \sqrt{\sum_{k=1,2} \sum_{l=1,2} \left[ \frac{\partial^2 \psi}{\partial x_k \partial x_l} \right]_i^2 + \epsilon \left[ \frac{\partial^2 \psi}{\partial x_k \partial x_l} \right]_i^2},
\]  

\( (3.120) \)

where \( \epsilon = 0.01 \) and the derivatives are evaluated using standard second order methods. A block is marked for refinement if \( E_{\max} > 0.8 \) and marked for derefinement if \( E_{\max} < 0.2 \).

### 3.6.3 PARAMESH

There are several freely available libraries that implement SAMR such as SAMRAI [161], Chombo [162], and PARAMESH [163–166] to name a few. In this work, the Paramesh library will be used. PARAMESH has been predominantly developed for and used by the astrophysics community to simulate events ranging from neutron star detonations [167] to the interaction of a cometary atmosphere with solar wind [168].
PARAMESH splits the domain into a hierarchy of sub-grids or blocks, which form the nodes of a quad tree data structure. When a block is tagged for refinement, the coarser parent block spawns four child blocks in 2-D. Each block is logically identical in shape, number of cells, aspect ratio, etc; however, the size, location, and list of neighbors, parents, and children are different for each block. Blocks containing the finest grid at a given location are called leaf blocks (the leaves of the tree). Each block has a ring of guard cells which are used as boundary conditions.

The main task when using PARAMESH is to develop a code that works on a single, uniform grid and to provide refinement/derefinement criterion. PARAMESH handles all of the communication, grid generation, parallelization, etc. As long as the PARAMESH functions and subroutines are properly used, a code developed for a single uniform grid can be ported to PARAMESH.

One of distinct advantages of PARAMESH over some of its competitors is that it scales very well on massively parallel architectures [166]. The feature that each block is logically identical makes the implementation of the level set method with PARAMESH far simpler in comparison to other libraries. If the refinement criterion around the interface and the number of guard cells are properly chosen, data will never be prolonged or restricted near the gas-liquid interface. Other libraries implement an agglomeration step to reduce the total number of blocks and minimize communication costs. Because of this, the scattered interpolation method of Nourgaliev et al. [44] must be used regardless of the refinement criterion and the number of guard cells if SAMRAI or Chombo are used.

Rather than utilizing PARAMESH to communicate the conserved variables as is commonly done, the strategy employed in this work is to use PARAMESH for keeping track of and communicating the primitive variables \((Y_1, Y_2, \ldots, Y_{N_g-1}, u, v, p \text{ and } T)\). The final mass fraction, \(Y_{N_g}\), is easily calculated from the constraint that \(\sum Y_i = 1\) and the density is calculated directly using the ideal gas equation of state. If the conserved variables were communicated instead, the multi-component equation of state would have to be inverted at all grid points including the values for all guard cells. This is very inefficient because inverting the equation of state for the parabolic operator is expensive and would have to be performed twice for many of the grid points. This would also necessarily decrease parallel efficiency since the values \(\gamma\) and \(\rho h_0^m\) would have to be communicated in addition to the conserved variables.
The formal conservative edge treatment, which is traditionally used with SAMR, is cumbersome to implement with the double flux model. It was found that no special edge flux treatment was necessary if the grid refinement is checked often enough to ensure that the stencils used to form the hyperbolic flux in coarse blocks never encounter a discontinuity that is located in a neighboring fine block. Grid refinement is checked in five time-step intervals using a layer of six guard cells, which gives coarser blocks sufficient warning to be refined before shock waves or contact discontinuities can influence them.

The overall steps for using AMR in this work goes as follows:

1. Calculate $\gamma$ and $\rho h_0^m$ on all interior cells, use zeroth order injection to populate guard cells for a one-cell ring, and store $\gamma$ and $\rho h_0^m$ for the entire hyperbolic step.

2. Invert the equation of state and calculate the primitive variables $Y_1, Y_2, \cdots, Y_{N_g-1}, u, v, p, T$ at the interior cells of each leaf block (which form the leaves in the quad-tree data structure).

3. Transfer the primitive variable array to PARAMESH’s data structure.

4. Use PARAMESH to fill values for the guard cells and apply boundary conditions.

5. Loop over all leaf blocks:
   (a) Calculate $Y_{N_g}$ and $\rho$ at the interior and guard cells.
   (b) Proceed using the single grid routines on the current block.

6. End Loop

The refinement criterion of Sun and Takayama [159] applied to density is used. A block is marked for refinement if $e_{\text{max}} = \max(e_{ij}) > \epsilon_{\text{ref}}$ and derefinement if $e_{\text{max}} < \epsilon_{\text{deref}}$. Unless otherwise noted, $\epsilon_{\text{ref}} = 0.03$ and $\epsilon_{\text{deref}} = 0.01$. A block can only be derefined if all of its siblings are marked for derefinement and its parent block is not marked for refinement. If child blocks were allowed to be derefined when the parent block was marked for refinement, derefinement/refinement flip-flops would occur with consecutive grid updates. This would cause a lot of unnecessary prolongation and can reduce the quality of the solution.

An example of PARAMESH used to calculate interaction of a Mach two shock wave with a 5.6 mm-diameter hydrogen bubble at a time of 8.8 $\mu$s is shown in Figure 3.9. The finest level of refinement corresponds to a 576×1728 cell grid and the refinement criterion of
3.7 Initialization

The initial conditions for the post-shock region of the domain are obtained by solving the Rankine-Hugoniot conditions:

\[
\begin{align*}
\rho_1(V_s - u_1) &= \rho_2(V_s - u_2), \\
p_1 + \rho_1(V_s - u_1)^2 &= p_2 + \rho_2(V_s - u_2)^2, \\
h_1(T_1) + \frac{(V_s - u_1)^2}{2} &= h_2(T_2) + \frac{(V_s - u_2)^2}{2},
\end{align*}
\] (3.121)

where \(V_s\) is the absolute shock velocity. States 1 and 2 refer to the pre- and post-shocked states, respectively. The post-shocked state is determined from the specified pre-shocked state and shock velocity or shock Mach number using Newton-Raphson iteration on the Rankine-Hugoniot conditions. The initial guess is calculated by using the analytical solution for the Rankine-Hugoniot conditions with constant properties:

\[
u_{2, \text{guess}} = u_1 + \frac{2}{\gamma + 1} \left[ \frac{(\sqrt{\gamma}RT_1 + u_1 - V_s)(\sqrt{\gamma}RT_1 - u_1 + V_s)}{u_1 - V_s} \right],
\] (3.122)
\[
\begin{align*}
p_{2, \text{guess}} &= p_1 + \rho_1(u_1 - u_2)(u_1 - V_s), \quad (3.123) \\
\rho_{2, \text{guess}} &= \frac{\rho_1 V_s - u_1}{V_s - u_2}. \quad (3.124)
\end{align*}
\]

Even when the shocked state is set properly, small startup errors are always produced [114]. These errors are quite small and have very little effect on the overall calculation. Since the startup error associated with a shock wave occurs regardless of whether the shock is spread over multiple computational cells or not, the initial shock profiles are not smeared.

Most of the conservation error produced by the double flux model occurs when numerical dissipation from the hyperbolic integration step mixes species at sharp contact surfaces. To reduce this problem, initial contact surfaces (unless otherwise noted) are smeared slightly. To initialize a function \( f \) in a bubble of diameter \( d \) at position \( r_o \) with function values of \( f_{\text{in}} \) and \( f_{\text{out}} \) inside and outside the bubble respectively, the following expression is used:

\[
f = \frac{f_{\text{out}} + f_{\text{in}}}{2} - \frac{f_{\text{out}} - f_{\text{in}}}{2} \tanh \left[ C_r \left( \frac{d}{2} - |r - r_o| \right) \right].
\]

(3.125)

The parameter \( C_r \) is a smearing parameter that is set to a value which spreads the contact surface over eight or nine computational cells, which is around the number of cells that the higher-order edge interpolation schemes tend to dissipate a contact surface.
4.1 Derivation

The following discussion closely follows Sethian [54]. Consider a domain, \( \Omega \), which is divided this domain into two regions denoted as \( \Omega^+ \) and \( \Omega^- \) with a boundary \( \partial \Omega \) separating the two sub regions:

\[
\Omega^+ \subseteq \Omega \quad \text{and} \quad \Omega^- \subseteq \Omega.
\] (4.1)

Now define an implicit function \( \phi \) that is equal to zero only on \( \partial \Omega \). To make \( \phi \) even more useful, let \( \phi \) be less than zero in \( \Omega^- \) and greater than zero in \( \Omega^+ \). Without a loss of generality, assume the surface, \( \partial \Omega \), is propagating locally with some speed \( \mathbf{V}_n \) in the normal direction as shown in Figure 4.1. The motion of the surface, in general, is a function of three broad items: local geometric properties of the surface, \( L \), such as curvature and the surface normal; global properties of the front, \( G \), that depend on the shape and position; and properties that are independent of the surface, \( I \), such as advection.

To derive an evolution equation for the level set function, \( \phi \), we assume that its motion, in general, is a function of both position and time. Thus, using the above definitions, the equation of \( \partial \Omega \) is:

\[
\phi (\mathbf{x}(t), t) = 0.
\] (4.2)
Using the chain rule, we get:
\[
\frac{\partial \phi}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla \phi = 0,
\]
where \( \mathbf{x}'(t) \) is the general speed function of the boundary. Thus, we have a scalar wave equation describing the motion of the surface.

In fluid mechanical applications, the surface moves at the local fluid velocity, \( \mathbf{u} \), and/or it moves normal to itself when undergoing phase change with velocity \( u_n \). Neglecting curvature effects, the equation of motion for the surface is:

\[
\frac{\partial \phi}{\partial t} + (\mathbf{u} + u_n) \cdot \nabla \phi = 0,
\]
where \( u_n \) represents the normal velocity at the surface due to phase change. Then

\[
u_n = -r_b \mathbf{n} = -r_b \frac{\nabla \phi}{|\nabla \phi|}.
\]

### 4.2 Signed Distance Functions

Little was stated about the level set function other than it being zero on the surface, positive on one side, and negative on the other side. For numerical reasons, it is an advantage if \( \phi \) is defined to be a continuous function. It would be of additional use if the value of the level set function was meaningful in some capacity.
Given a boundary \( \partial \Omega \), we define the distance function \( d(x) \) as [55]:

\[
d(x) = \min (|x - x_1|) \quad \forall x_1 \in \partial \Omega,
\]

where \( x_1 \) is the position vector of any point on the surface. Geometrically, the value of \( d(x) \) represents the distance from a point to the nearest location on the surface. The distance function is simply a Euclidean distance with the following important property:

\[
|\nabla d| = 1.
\]

(4.7)

The signed distance function (or level set function), \( \phi \), is a generalization of the distance function that changes sign depending on which sub-domain a point is located:

\[
\phi(x) = \begin{cases} 
  d(x) & \forall x \in \Omega^+ \\
  -d(x) & \forall x \in \Omega^- \\
  0 & \forall x \in \partial \Omega.
\end{cases}
\]

(4.8)

Thus, the magnitude of the signed distance function tells how far a given point is from the surface and the sign of the signed distance function indicates in which sub-domain the point is located. It is clear from its definition that \( \phi \) is a continuous and smooth function except near kinks where it is non-differentiable. Most numerical methods will smooth out non-differentiable points. An example of a surface and its corresponding signed distance function is shown in Figure 4.2.

### 4.3 Initialization and Reinitialization

Given initial surface data, how can the signed distance function be formed? A naïve approach is to seed the surface with many points and use Eq. (4.8) directly. This approach, while exact, is computationally time consuming. A faster and more elegant approach is to solve the reinitialization equation, \( |\nabla \phi| = 1 \). A solution to this Eikonal equation is needed, which is highly non-linear and exceedingly to directly difficult solve. The Eikonal equation can be solved much more simply using a pseudo-time stepping approach by marching:

\[
\frac{\partial \phi}{\partial \tau} + |\nabla \phi| - 1 = 0
\]

(4.9)
Figure 4.2: Shape of a surface (left) and its signed distance function (right).

to steady-state. If Eq. (4.9) is marched directly, all of the information will travel in one
direction and the zero of the level set function will move, destroying the surface information.
Care must be taken to avoid this so that a signed distance function is formed. Thus, Eq. (4.9)
is slightly modified to

\[ \frac{\partial \phi}{\partial \tau} + \text{sgn}(\phi) (|\nabla \phi| - 1) = 0, \]

where \( \text{sgn}(\phi) \) is the signum function:

\[
\text{sgn}(\phi) = \begin{cases} 
-1 & \phi < 0 \\
1 & \phi > 0 \\
0 & \phi = 0.
\end{cases}
\]

This ensures that signed distance function “waves” will be generated from the surface and
travel away from it, while leaving the surface alone. In practice, a smoothed signum function
[169] is used to avoid wrinkling the surface:

\[
\text{sgn}(\phi) = \frac{\phi}{\sqrt{\phi^2 + \max(\Delta x, \Delta y)^2 |D(\phi)|^2}},
\]

(4.12)
where $D(\phi)$ is the spatial operator used in solving Eq. (4.10).

Solving the Eikonal equation is not only useful for providing an initial level set function, but also for smoothing the level set function throughout the advancement of Eq. (4.4). As a surface is evolved, a generic velocity field may not preserve the properties of the signed distance function. Even though this work is primarily interested in the location of the zero level set for fluid mechanics calculations, care must be taken to ensure that error occurring during the advancement of the signed distance function does not lead to any discontinuities or ruin the calculation of the surface normal vector and curvature. This error is alleviated by solving the reinitialization equation after a number of time steps to eliminate any errors of the level set by returning it to a signed distance function.

4.4 Solution Methods for the Level Set Equation

The Hamilton-Jacobi (HJ) equation for the signed distance function, $\phi$, is:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi + u_n|\nabla \phi| = 0.$$  \hfill (4.13)

4.4.1 Motion in an External Velocity Field

The discretization of the advection portion of the HJ equation, 

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0,$$  \hfill (4.14)

is similar to solving a conservation law, with the exception that the steps are performed in the opposite order. The steps in solving conservation laws are to interpolate variables to cell edges, form the fluxes, and finally calculate the flux gradient at the cell center by taking the divided difference of the edge flux values. When solving Hamilton-Jacobi equations, the divided differences, $D_{i+1/2,j} = \phi_{i+1,j} - \phi_{i,j}$, are first formed at the cell edges from the cell center values. The divided differences are interpolated from the cell edges to the cell center in the upwind direction ($D_{L,i}$ or $D_{R,i}$) using any of the interpolation schemes presented in Appendix B. After the interpolation of the divided difference the cell-centered divided
difference is multiplied by the velocity at the cell center to form:

\[
 u\phi_x|_i = \frac{1}{\Delta x} \begin{cases} 
 u_i D_{L,i} & \text{if } u_i \geq 0 \\
 u_i D_{R,i} & \text{if } u_i < 0.
\end{cases}
\]

(4.15)

The method of lines is used to integrate the level set equation using second-order Runge-Kutta. In the event that the value of the level set function at a cell center becomes exactly zero (typically during initialization), it is given a slightly positive value. Discretization in other directions is similar.

In many cases the local fluid velocity, \( \mathbf{u} \), can simply be used to move the level set function. However, velocity is not continuous near the interface with calculations involving compressible flows, shock waves, and/or phase change. Using the local fluid velocity in the HJ equation would result in the level function no longer being a signed distance function and possibly cause unwanted motion of the surface. The unwanted motion of the zero level set can be minimized by extrapolating the velocity of the interface across the surface.

### 4.4.2 Motion in the Normal Direction

The HJ equation for motion in the normal direction is:

\[
 \frac{\partial \phi}{\partial t} + u_n H_n(\phi) = 0,
\]

(4.16)

where \( H_n(\phi) = \sqrt{\phi_x^2 + \phi_y^2} \) in two dimensions. It is quite difficult to derive advection schemes to solve this equation as is, thus the advection term is multiplied by \( |\nabla \phi|/|\nabla \phi| \), giving:

\[
 \frac{\partial \phi}{\partial t} + \frac{u_n \phi_x}{\sqrt{\phi_x^2 + \phi_y^2}} \phi_x + \frac{u_n \phi_y}{\sqrt{\phi_x^2 + \phi_y^2}} \phi_y = 0,
\]

(4.17)

which is in a form that Godunov’s method for non-linear equations can be applied. Osher and Fedkiw [55] recommend the following Godunov scheme. The quantities \( u_{n,i} D_{L,i} \) and \( u_{n,i} D_{R,i} \) are calculated using the method described earlier on a direction-by-direction basis. Then the discretization of \( \phi_x \) is:

\[
 H_n(\phi) = \begin{cases} 
 \max(|(D_{R,x})^2|, |(D_{L,x})^2|) + \max(|(D_{R,y})^2|, |(D_{L,y})^2|) & \text{if } u_n > 0 \\
 \max(|(D_{R,x})^2|, |(D_{L,x})^2|) + \max(|(D_{R,y})^2|, |(D_{L,y})^2|) & \text{if } u_n \leq 0,
\end{cases}
\]

(4.18)
where \((a)^- = \min(a, 0)\) and \((a)^+ = \max(a, 0)\).

### 4.4.3 Fast Local Level Set Method

Peng et al. [169] noted that in many applications the level set function is only needed near the interface. In these situations, it is far more efficient to evolve the level set equation near the interface, within a tube of \(\zeta \Delta x\), but not far from the interface. To efficiently achieve this, Peng et al. [169] developed the Fast Local Level Set Method (FLLS), which multiplies the fluid velocity, \(u\), and the normal velocity, \(u_n\), by \(C(\phi)\):

\[
C(\phi) = \begin{cases} 
1 & \text{if } |\phi| \leq \beta \Delta x \\
\frac{2|\phi| + \Delta x(\zeta - 3\beta)}{(\zeta - \beta)^3 \Delta x^3}(|\phi| - \zeta \Delta x)^2 & \text{if } \beta \Delta x < |\phi| \leq \zeta \Delta x \\
0 & \text{if } |\phi| > \zeta \Delta x,
\end{cases} \tag{4.19}
\]

where \(\beta\) is the radius of an “inner tube” where the speed function is unmodified and \(\zeta\) is the radius of an “outer tube” where outside of this tube, the level set equation is not evolved. Using this modification, the fluid velocity and normal velocity used to evolve the signed distance function are \(u^{\text{mod}} = C(\phi)u\) and \(u_n^{\text{mod}} = C(\phi)u_n\), respectively. In locations where \(C(\phi) > \zeta \Delta x\) the level set equation is not evolved at all. In this work \(\beta = 7\) and \(\zeta = 10\).

### 4.5 Solution Method for the Reinitialization Equation

The Eikonal equation, \(|\nabla \phi| = 1\), is solved by marching:

\[
\frac{\partial \phi}{\partial \tau} + \text{sgn}(\phi)[H_n(\phi) - 1] = 0 \tag{4.20}
\]

to steady state using a pseudo time stepping approach, which is quite similar to discretizing motion in the normal direction, with the exception that \(u_n\) is replaced with \(\text{sgn}(\phi)\) in Eq. (4.18). The signum function is usually defined to be one of the following smeared versions:

\[
\text{sgn}(\phi^0) = \frac{\phi^0}{\sqrt{(\phi^0)^2 + \Delta x^2}}, \tag{4.21}
\]
\[
\text{sgn}(\phi) = \frac{\phi}{\sqrt{(\phi^0)^2 + |\nabla \phi|^2 \Delta x^2}}, \tag{4.22}
\]
where $\phi^0$ is the initial guess for the signed distance function. The first signum function only evaluates the sign of the level set function using the initial guess for the signed distance function. The later version of the smeared signum function is more robust and works better if the initial guess for the signed distance function is very poor, but needs to be constantly reevaluated as the development of the signed distance function progresses. As pointed out earlier, the reinitialization equation is only used to initialize the level set function and to return the level set function to a signed distance function if ripples and sharp gradients are formed as it moves. Thus, it is overkill to use very high-order schemes since the calculation only needs information on the level set function near the interface.

In this work, the reinitialization method of Min and Gibou [170] is used. First they define:

$$D^0_x \phi_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x},$$

$$D^0_{xx} \phi_i = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}.$$  \hspace{1cm} (4.23)

Using these definitions, the divided differences in the x-direction, $D_x$, are:

$$D_{L,i} = \frac{\phi_i - \phi_{i-1}}{\Delta x} - \frac{\Delta x}{2} \minmod(D^0_{xx} \phi_i, D^0_{xx} \phi_{i-1}),$$

$$D_{R,i} = \frac{\phi_{i+1} - \phi_i}{\Delta x} + \frac{\Delta x}{2} \minmod(D^0_{xx} \phi_i, D^0_{xx} \phi_{i+1}),$$ \hspace{1cm} (4.24)

where

$$\minmod(a, b) = \begin{cases} 
\max(a, b) & \text{if } a < 0 \text{ and } b < 0 \\
\min(a, b) & \text{if } a > 0 \text{ and } b > 0 \\
0 & \text{otherwise.}
\end{cases}$$ \hspace{1cm} (4.25)

The divided differences are used to discretize $H_n(\phi)$ for the reinitialization equation using Eq. (4.18) with the exception that $u_n$ is replaced with $\text{sgn}(\phi)$.

One issue with reinitialization procedure is that the motion of the zero level set will move slightly as the reinitialization equation is marched to steady state. Min and Gibou [170] minimize this problem by altering the divided difference when the zero of the level set function lies between grid points. If $\phi_i \phi_{i+1} < 0$, the interface lies between grid points $i$ and $i + 1$. The distance between the interface and $x_i$, $s_I$, is estimated using quadratic
interpolation:

\[ s_I = \frac{\Delta x}{2} + \begin{cases} 
-c_0/c_1 & \text{if } |c_2| < \epsilon \\
(-c_1 + \sqrt{c_1^2 - 4c_2c_0})/(2c_2) & \text{if } |c_2| \geq \epsilon \text{ and } \phi^0_i < 0 \\
(-c_1 - \sqrt{c_1^2 - 4c_2c_0})/(2c_2) & \text{if } |c_2| \geq \epsilon \text{ and } \phi^0_i < 0,
\end{cases} \tag{4.26} \]

where

\[ c_2 = \frac{1}{2} \minmod(D_{xx}^0 \phi^0_i, D_{xx}^0 \phi^0_{i+1}), \]
\[ c_1 = \frac{\phi^0_{i+1} - \phi^0_i}{\Delta x}, \]
\[ c_0 = \frac{\phi^0_{i+1} + \phi^0_i}{2} - \frac{\Delta x c_2^2}{4}, \]

and \( \phi^0 \) is the value of the initial level set function. The divided difference in the cut cell is:

\[ D_{R,i} = \frac{0 - \phi^n_i}{s_I} + \frac{s_I}{2} \minmod(D_{xx}^0 \phi_i, D_{xx}^0 \phi_{i+1}). \tag{4.27} \]

The cut cell does not affect \( D_{L,i} \), but it influences \( D_{L,i+1} \). When the interface lies between grid points \( i \) and \( i+1 \), \( s_{I,i+1} = \Delta x - s_{I,i} \) and

\[ D_{L,i+1} = \frac{\phi^n_{i+1} - 0}{s_{I,i+1}} - \frac{s_{I,i+1}}{2} \minmod(D_{xx}^0 \phi_i, D_{xx}^0 \phi_{i+1}). \tag{4.28} \]

The time step restriction for the cut cells is:

\[ \Delta \tau = \min(s_I, \Delta x, \Delta y)/2. \tag{4.29} \]

Since steady state is required for the reinitialization equation, the above time step restriction is applied locally for each cell, rather than globally. Second-order Runge-Kutta is used to advance \( \phi \) from time level \( n \) to \( n + 1 \) during reinitialization.

### 4.6 Extrapolation Across the Interface

In many situations it is necessary to extrapolate some variables across the interface. In this work the partial differential equation approach of Aslam [171] is used. The PDE to achieve
constant extrapolation of a variable $\psi$ across the interface in the normal direction is:

$$\frac{\partial \psi}{\partial \tau} + H(\phi) \hat{n} \cdot \nabla \psi = 0,$$

(4.30)

where

$$\hat{n} = \frac{\nabla \phi}{|\nabla \phi|}.$$  

(4.31)

$H(\phi)$ is a Heaviside function whose definition depends on the type of extrapolation being performed [171, 172]. When extrapolating data from the negative side to the positive side,

$$H(\phi) = \begin{cases} 
0 & \text{if } \phi \leq 0 \\
1 & \text{if } \phi > 0. 
\end{cases}$$

(4.32)

When extrapolating data from the positive side to the negative,

$$H(\phi) = \begin{cases} 
-1 & \text{if } \phi \leq 0 \\
0 & \text{if } \phi > 0. 
\end{cases}$$

(4.33)

When extrapolating a variable that is only defined on the interface to both regions,

$$H(\phi) = \begin{cases} 
-1 & \text{if } \phi < 0 \\
0 & \text{if } \phi = 0 \\
1 & \text{if } \phi > 0. 
\end{cases}$$

(4.34)

In two dimensions the Hamiltonian for the extrapolation equation, $H_E = H(\phi) \hat{n} \cdot \nabla \psi$, is discretized using a first-order upwind scheme:

$$H_{E,i,j} = \max[H(\phi_{i,j}) \hat{n}_{x,i,j}, 0] \frac{\psi_{i,j} - \psi_{i-1,j}}{\Delta x} + \min[H(\phi_{i,j}) \hat{n}_{x,i,j}, 0] \frac{\psi_{i+1,j} - \psi_{i,j}}{\Delta x}$$

$$+ \max[H(\phi_{i,j}) \hat{n}_{y,i,j}, 0] \frac{\psi_{i,j} - \psi_{i,j-1}}{\Delta y} + \min[H(\phi_{i,j}) \hat{n}_{y,i,j}, 0] \frac{\psi_{i,j+1} - \psi_{i,j}}{\Delta y},$$

(4.35)

where $\hat{n}_x$ and $\hat{n}_y$ are the x and y components of the normal direction.

The extrapolation is then marched in pseudo-time using the second-order TVD Runge-Kutta scheme discussed above for the reinitialization equation. Linear, quadratic, and even
higher-order PDE extrapolation methods have been formulated [171], but were not used due to their expense.

4.7 Calculation of Surface Area and Volume

It is often of interest to calculate quantities such as the surface area and volume of a region. Following Osher et al. [55], volume integrals and surface integrals can be calculated using multidimensional Heaviside and Dirac delta functions. The volume integral of \( f(x) \) on \( \Omega^+ \) is defined as:

\[
\iiint_{\Omega^+} f(x) \, d\Omega^+ = \iiint_{\Omega} f(x) H(\phi(x)) \, d\Omega. \tag{4.36}
\]

The Heaviside function, \( H \), in Eq. (4.36) zeros out any data that is not in \( \Omega^+ \). Similarly, the volume integral in the negative region is:

\[
\iiint_{\Omega^-} f(x) \, d\Omega^- = \iiint_{\Omega} f(x) \left[ 1 - H(\phi(x)) \right] \, d\Omega. \tag{4.37}
\]

When the quantity of interest is a surface integral, the Dirac delta function must be utilized. By definition, the multidimensional Dirac delta function, \( \delta(x) \), is:

\[
\delta(x) = \nabla H(\phi(x)) \cdot \hat{n}. \tag{4.38}
\]

Using the chain rule:

\[
\delta(x) = H'(\phi(x)) \nabla \phi(x) \cdot \frac{\nabla \phi(x)}{\left| \nabla \phi(x) \right|} = H'(\phi(x)) \left| \nabla \phi(x) \right|. \tag{4.39}
\]

By definition \( \delta(\phi) = H'(\phi) \), thus the surface integral is:

\[
\iint_{\partial \Omega} f(x) \, dA = \iiint_{\Omega} f(x) \delta(\phi(x)) \, d\Omega = \iint_{\Omega} f(x) \delta(\phi(x)) \left| \nabla \phi(x) \right| \, d\Omega = \iiint_{\Omega} f(x) \delta(\phi(x)) \, d\Omega. \tag{4.40}
\]
The last step in Eq. (4.40) was made by using the Euclidean distance property of the signed distance function.

Using numerical approximations, the signed distance function is known only at discrete locations. To facilitate first-order accurate integration, the smeared Heaviside and Dirac delta functions can be used. To evaluate volume and surface integrals, the smeared Heaviside function is:

\[
H(\phi) = \begin{cases} 
0 & \text{if } \phi < -\epsilon \\
\frac{1}{2} + \frac{\phi}{2\epsilon} + \frac{1}{2\pi} \sin\left(\frac{\pi \phi}{\epsilon}\right) & \text{if } -\epsilon \leq \phi \leq \epsilon \\
1 & \text{if } \phi > \epsilon,
\end{cases}
\] (4.41)

and the smeared Dirac delta function is:

\[
\delta(\phi) = \begin{cases} 
0 & \text{if } \phi < -\epsilon \\
\frac{1}{2\epsilon} + \frac{\phi}{2\epsilon} \cos\left(\frac{\pi \phi}{\epsilon}\right) & \text{if } -\epsilon \leq \phi \leq \epsilon \\
0 & \text{if } \phi > \epsilon.
\end{cases}
\] (4.42)

As an example, the signed distance function and surface area of a cylindrical propellant grain and a comparison of burning surface area as a function of \(\phi\) (or the web distance) evaluated using Huygens principle and the level set method using the smeared Dirac delta function. The signed distance function of a star propellant grain was calculated and as shown.
Figure 4.4: Calculated (a) signed distance function for a star propellant grain using a 400 by 400 grid and (b) the burning perimeter as a function of $\phi$.

in Figure 4.4 along with the burning perimeter of the propellant as a function of burn back distance.

Integration of surface and volume quantities during a practical calculation using the smear Heaviside and Dirac delta functions can be quite expensive. For example, to integrate the rate of mass transfer from a surface, surface mass flux would have to be extrapolated in both directions. To evaluate the integrals more quickly, the above integration techniques are not used and the volume integral of a particular fluid is simply:

$$
\int\int\int_{\Omega^+} f(\mathbf{x}) d\Omega^+ \approx \sum_{\text{cells}} f_{i,j} V_{i,j} \max[0, \text{sgn}(\phi_{i,j})],
$$

$$
\int\int\int_{\Omega^-} f(\mathbf{x}) d\Omega^- \approx \sum_{\text{cells}} f_{i,j} V_{i,j} \max[0, -\text{sgn}(\phi_{i,j})].
$$

Note that the volume of cut-cells are not accounted for. Surface integrals of scalar quantities that are assumed to be in the normal direction (e.g., mass flux from vaporization) are approximated as:

$$
\int\int f(\mathbf{x}) \approx \sum_{\text{edges}} f |\hat{n} \cdot \hat{n}_{\text{face}}|.
$$
where the surface function, $f$, is defined to be non-zero only along the surface. These approximations may be crude, but incurred less than 1% error when a circle was discretized with 120 points across the diameter.

### 4.8 Level Set Verification Tests

To ensure proper implementation of the level set method itself, several verification tests were performed including Zelasak’s circle and the two-dimensional stretching and deformation of a circular cylinder. Both calculations are performed on the unit square using a 512×512 grid and discretization was performed using fifth-order non-linear error-controlled WENO. The level set equation was advanced in time using RK2 with a CFL number of unity.

The first test is the counter-clockwise solid body rotation of a slotted circle (often called Zelasak’s circle) of radius 0.15 m centered at $x = 0.5$ m and $y = 0.75$ m. The length and width of the slot were 0.25 m and 0.05 m, respectively. The interface was advanced for one full revolution and its evolution is shown in Figure 4.5. Due to numerical dissipation, the initially sharp edges become smooth (as shown in Figure 4.6). As a result, a little over 0.3% of the area inside Zelasak’s circle is lost.

A more severe numerical experiment is the two-dimensional stretching and deformation test. A circle of radius 0.15 m is centered at $x = 0.5$ m and $y = 0.75$ m. Rather than applying a solid body rotation the velocity field is given by:

$$
\begin{align*}
    u &= -2 \cos\left(\frac{\pi t}{2}\right) \cos(\pi y) \sin^2(\phi x) \sin(\pi y), \\
    v &= 2 \cos\left(\frac{\pi t}{2}\right) \cos(\pi x) \sin^2(\phi y) \sin(\pi x).
\end{align*}
$$

This flow field massively deforms and stretches the interface until the flow field reverses at $t = 2$ s. At $t = 4$ s the interface should return exactly to its original position; however, due to numerical dissipation and dispersion errors this is not the case. The time evolution of the deforming cylinder is shown in Figure 4.7. A comparison of the initial and final shapes and percent area loss is shown in Figure 4.8.

Other numerical experiments, such as the oscillation of a circle, were also performed and are not presented for the sake of brevity.
4.9 Coupling the Gas and Liquid Regions

The numerical methods previously described only deal with solving the conservation equations in their respective regions and moving the interface between the gas and liquid regions. Methods such as the ghost fluid method [55, 67, 74, 173–175] or cut-cell based methods [44, 57, 176–179] are needed to couple the gas and liquid regions.

4.9.1 Cut Cell Methods

Cut-cell based methods, such as the adaptive characteristics based matching method [44] or the sharp interface method (SIM) [176, 177], use the level set function to cut cells at the interface into two cells that contain one fluid or the other. The flow variables are extrapolated
to the gas and liquid sides of the interface, where jump conditions are calculated and then applied at the cell edge. In some variants the cells containing the interface are cut on a directional basis, essentially stair-stepping the interface. The jump conditions and/or a solution to the two-phase Riemann problem are calculated at the edges of the cut cells and used to locally fill the ghost cells [44, 57].

In other variants [176–179] the intersection of the zero level set and the cell edges are used to cut the cells in a multi-dimensional manner, forming an unstructured mesh near the interface. Variables are interpolated to the edges and centroid of the cut cells using some form of scattered multi-dimensional interpolation, such a least-squares based interpolation or Shepard’s interpolation [156–158]. The fluxes at the cut cell edges are calculated using the jump conditions and the conserved variables at the centroid of the cut cell. After time advancement, the variables at the cut cells are re-interpolated back to the original mesh and the unstructured cut-cell mesh is destroyed. This process repeats itself every time step.

Cut-cell methods have the advantage of producing a very sharp interface, but can be complicated to implement. First a meshing algorithm must be implemented to form the cut cells. Very small cut cells are agglomerated with neighboring cells to avoid an overly restrictive time step. The meshing process in two-dimensions may not be too difficult; however, using these methods in three dimensions requires surface-based meshing methods,
4.9.2 Ghost Fluid Method

The ghost fluid method (GFM) keeps track of two sets of conserved variables, real and ghost variables. The real variables correspond to the values in the region where they belong (e.g., gas-phase primitive variables in the gas-phase region) and the ghost variables correspond to data across the interface (e.g., gas-phase variables in the liquid region). Once the ghost cells are filled, the calculation proceeds as normal, with the exception that the ghost cells are used in the stencils near the interface. Cells cut by the interface are treated identically, with the exception that the sign of the level set function in the cut cell dictates which set of conservation laws to advance.

Originally the GFM was applied to the Euler equations with compressible gases and liquids [67]. Coupling two inviscid regions is complicated by the fact that not all of the variables are continuous and there are not enough relations to provide jump conditions for all variables. In the absence of viscous effects, phase change, and surface tension the following jump conditions hold: \([u_n] = 0\) and \([p] = 0\). However, the jump relations for tangential momentum and energy do not provide any information for inviscid flows. In their
seminal work, Fedkiw et al. [67] devised a clever work-around to this problem and developed the GFM.

In the first iteration of the GFM, the ghost values of the pressure and the normal velocity were simply copied from the real fluid values, while the tangential velocity was extrapolated across the interface. Since there are not enough jump conditions for inviscid flow to use an equation of state in the ghost region, Fedkiw et al. [67] apply an isobaric fix [173] by extrapolating an isobaric fix variable—such as entropy—across the interface. Density in the ghost region was obtained by using the equation of state, the ghost pressure, and the isobaric fix variable. An illustration of this filling procedure (sometimes called soft coupling) is shown in Figure 4.9.

The practice of filling ghost values of pressure and velocity by directly copying from the ghost region works well for low density ratios between the two regions, but leads to large overheating errors (i.e., a sharp temperature spike) at the material interface for high density ratios. The key to reducing this error, introduced by Fedkiw [180], is to think of the interface as separating “stiff” and “soft” regions. The pressure in the ghost region of the stiff fluid is still directly copied from the soft fluid, but the normal velocity in the ghost region is extrapolated across the interface rather than directly copied. Conversely, the pressure in the ghost region of the soft fluid is extrapolated while the normal velocity directly copied. An illustration of this stiff coupling method is shown in Figure 4.10.
One drawback to ghost fluid methods is they do not correctly treat the Riemann problem at the interface. The original ghost fluid method with soft or stiff coupling actually solves two Riemann problems [73]. For example, in the case of compressible gas-liquid flow a gas-gas Riemann problem is solved when advancing the gas phase and a liquid-liquid Riemann problem is solved when advancing the liquid phase. This practice often leads to incorrect waves being reflected at the surface. For example, in some situations the GFM will predict a
reflected shock wave when it should actually be a rarefaction wave. Liu et al. [74] solved this problem by using the solution of the interfacial Riemann problem to populate ghost cells. They called their method the modified ghost fluid method (MGFM) and more recently developed a robust variant called the real ghost fluid method (rGFM) [75]. The MGFM and rGRM have even been successfully used to couple compressible, cavitating liquids [76, 181] with solids and gases. The interface Riemann solver developed for rGFM and MGFM is based on the two-shock approximate Riemann solver, which assumes that the characteristic waves traveling at velocity $u_I + c$ and $u_I - c$ are both shocks and that the interface moves with the contact surface at velocity $u_I$. In this work the rGFM method is adopted with the exception that the exact Riemann solution at the interface is utilized rather than an approximate solution.

4.9.3 The Riemann Problem at a Multi-fluid Interface

Consider the Riemann problem shown in Figure 4.11. Pressure and velocity are both constant across a contact surface for standard Riemann problems. When the effect of phase change and surface tension are considered, normal velocity and pressure are no longer constant across the contact surface (i.e., the gas-liquid interface) and jump conditions $J_C$ for pressure and velocity needs to be applied across the contact surface. These jump conditions are given using Eqs. (2.65) and (2.71). Assuming the normal vector is to the right and liquid phase is on the left side of the interface, the pressure and normal velocity in the starred states adjacent to the interface are related to the left and right states by:

\[
\begin{align*}
    u_I &= u^*_L - r_b, \\
    u^*_R &= u^*_L + [u], \\
    p^*_R &= p^*_L + [p].
\end{align*}
\]

(4.47)  
(4.48)  
(4.49)

Following the standard solution of the Riemann problem for gases [113] and liquids [182], the velocity of the contact surface can be calculated from the left and right states:

\[
\begin{align*}
    u_I &= u_L - r_b - f_L(p^*_L, u_L, p_L, \rho_L), \\
    u_I &= u_R - r_b - [u] + g_R(p^*_L + [p], u_R, p_R, \rho_R),
\end{align*}
\]

(4.50)  
(4.51)
where $f_L$ and $g_L$ represent velocity jump functions across the left and right waves. Combining the above equations, an implicit equation for the liquid pressure adjacent to the interface is derived:

$$f_L(p_L^*, u_L, p_L, \rho_L) + g_R(p_L^* + [p], u_R, p_R, \rho_R) + u_R - u_L - [u] = 0, \quad (4.52)$$

which is solved using Newton’s method. Even though the gas-phase region is a multi-component mixture with variable specific heat ratio, the double flux model essentially freezes the specific heat ratio and reference energy in each computational cell, treating it like a single-component constant-property ideal gas. Thus, the standard velocity jump functions presented in Toro [113] can be used without modification:

$$g_R = \begin{cases} 
(p_L^* + [p] - p_R) \sqrt{\frac{2}{(\gamma+1)\rho_R}} & \text{if } p_R < p_R^* \quad \text{(shock wave)} \\
\frac{2c_R}{\gamma-1} \left[ \left( \frac{p_L^* + [p]}{p_R} \right)^{\frac{\gamma+1}{\gamma-1}} - 1 \right] & \text{if } p_R \geq p_R^* \quad \text{(rarefaction wave).}
\end{cases} \quad (4.53)$$

The derivative of the right velocity jump function needed for Newton’s method is:

$$\frac{dg_R}{dp_L} = \begin{cases} 
\frac{g_R}{p_L^* + [p] - p_R} \left[ 1 - \frac{p_L^* + [p] - p_R}{2 \left( \frac{\gamma+1}{\gamma-1} p_R + p_L^* + [p] - p_R \right)} \right] & \text{if } p_R < p_R^* \\
\frac{1}{\rho_R c_R} \left( \frac{p_L^* + [p]}{p_R} \right)^{-\frac{\gamma+1}{\gamma-1}} & \text{if } p_R \geq p_R^*.
\end{cases} \quad (4.54)$$
For a barotropic fluid the velocity jump function is given by:

\[
\begin{align*}
  f_L &= \begin{cases} 
    \sqrt{\frac{p_L - p_L^*}{\rho_L^* - \rho_L}} & \text{if } p_L < p_L^* \quad \text{(shock wave)} \\
    \int_{p_L^*}^{p_L} \frac{dp}{\rho c} & \text{if } p_L \geq p_L^* \quad \text{(rarefaction wave)},
  \end{cases}
\end{align*}
\]

with derivatives

\[
\frac{df_L}{dp_L^*} = \begin{cases} 
    \frac{1}{2f_L} \left( \frac{1}{\rho_L} - \frac{1}{\rho_L^*} + \frac{p_L^* - p_L}{(\rho_L c_L^*)^2} \right) & \text{if } p_L < p_L^* \\
    \frac{1}{\rho_L c_L^*} & \text{if } p_L \geq p_L^*.
  \end{cases}
\]

If \( p_L \geq p_L^* \geq p_{\text{sat}} \) the fluid in the liquid region is not cavitating and the integral for a rarefaction wave can be computed analytically to give:

\[
f_L = \frac{2c_L}{N - 1} \left[ \left( \frac{p_L^* + B - A}{p + B - A} \right)^{\frac{N-1}{2N}} - 1 \right].
\]

If some or all of the fluid in the rarefaction wave is cavitating, the integration is performed approximately using Gaussian quadrature with eight points and the pressure split into sub-intervals. The error tolerance for the Newton-Raphson scheme is \( 10^{-12} \) and usually converges in around five or six iterations. For stability it was found that the values for the left and right Riemann states should be taken directly from adjacent cells, reducing the accuracy to first-order at the interface.

Species mass fractions and tangential velocity are Riemann invariants and do not change across shock or rarefaction waves. Thus, values of the species mass fractions in the right starred state are identical to the right state and the Riemann solution provides a condition on the total mass flux, but cannot provide information on the chemical species composition. If vaporization in a multi-component gas is to be considered, the parabolic step must be included to properly couple species mass and energy.

In one dimension, the starred states of the interfacial Riemann problem are used to populate ghost cells directly, as shown in Figure 4.12. In two dimensions the procedure for filling ghost cells is more complicated since there are two velocity components to consider and the interface is generally not aligned with the grid. Consider Figure 4.13, all computational cells that border the interface are identified by checking the sign of the level set function between neighboring cells along the x- and y-directions. Two adjacent cells border the
interface if $\phi_{ij} = \phi_A \phi_B \leq 0$. Next the normal vector,

$$\hat{n} = \frac{\nabla \phi}{|\nabla \phi|},$$

is calculated at the cell center of each cell using second-order central differencing. In some cases the normal vector calculated at an interfacial cell may be opposite to the signs of the level set function (see Figure 4.14). When this situation occurs, the normal vector at a cell edge is recalculated using first-order differencing in the direction normal to the cell face. If this situation does not occur, curvature and the normal vector are linearly interpolated to the interface position using:

$$f_{\text{interface}} = (1 - \theta)f_{i,j} + \theta f_{i+1,j},$$
where
\[ \theta = -\frac{\phi_{i,j}}{\phi_{i+1,j} - \phi_{i,j}}. \]  
(4.60)

For the purposes of more accurately computing the regression rate, the mass fractions at the interface, \( Y_{\text{interface}} \), are are estimated via:

\[
Y_{\text{interface}} = \begin{cases} 
Y_{i+1,j} - (1 - \theta)(Y_{i+2,j} - Y_{i+1,j}) & \text{if } \hat{n}_x > 0 \text{ and } \phi_{i+2,j} \geq 0 \\
Y_{i+1,j} & \text{if } \hat{n}_x > 0 \text{ and } \phi_{i+2,j} < 0 \\
Y_{i-1,j} + (1 - \theta)(Y_{i,j} - Y_{i-1,j}) & \text{if } \hat{n}_x < 0 \text{ and } \phi_{i-1,j} \geq 0 \\
Y_{i-1,j} & \text{if } \hat{n}_x < 0 \text{ and } \phi_{i-1,j} < 0.
\end{cases}
\]  
(4.61)
The velocities normal and tangential to the interface are:

\[
  u_n = \langle u, v \rangle \cdot \hat{n} = u\hat{n}_x + v\hat{n}_y
\]

\[
  u_t = \langle u, v \rangle \cdot \hat{t} = v\hat{n}_x - u\hat{n}_y.
\]

The interfacial Riemann problem at each cell edge of an interfacial is solved using pressure, density, and normal velocity from the cell centers of the cut-cells.

In the event that a cell is used in the calculation of two or more Riemann problems (such as the cell marked B in Figure 4.13) the final ghost state is taken as a weighted average all the interfacial Riemann solutions:

\[
  U = \frac{\sum_{i=1}^{N_{RS}} U_i |\hat{n} \cdot \hat{n}_{\text{cell face}}|}{\sum_{i=1}^{N_{RS}} |\hat{n} \cdot \hat{n}_{\text{cell face}}|},
\]

where \( N_{RS} \) is the number of times a cell was used in the solution of a interfacial Riemann problem, \( \hat{n}_{\text{cell face}} \) is the normal vector of the cell face, \( U \) is the final ghost state at the interfacial cell, and \( U_i \) is the solution for each individual Riemann problem.

Once all of the border Riemann problems have been solved, the pressure, density, temperature, velocity components, and species mass fractions are extrapolated in the normal direction into the ghost region for each fluid using the PDE-based methods discussed above. Finally, the calculation of the cell edge fluxes can proceed as usual after the ghost cells have been filled. For stability purposes the interfacial liquid-phase flux calculated directly from the averaged Riemann solution rather than using a Rusanov or LLF flux evaluation scheme.

The flux evaluation procedure outlined in Chapter 3 is utilized for the gas phase.

Using block structured AMR, the procedure for filling the ghost cells is slightly more complicated. If done improperly, the extrapolated states on blocks sharing the same edge may be different and possibly ruin the calculation. To avoid this, Riemann problems are solved not only on the interior cells of a block, but also on the guard cells. The extrapolation is then performed on both the interior and guard cells locally on each block for nine iterations. This procedure solves many duplicate interfacial Riemann problems, but has relatively little dependence on the size and position of the AMR blocks and significantly reduces communication and synchronization costs compared to filling the ghost cells globally.
4.9.4 Interfacial Riemann Problems with Exact Solutions

To ensure that the interface coupling technique is accurate and properly implemented, several interfacial Riemann problems were calculated and compared with exact solutions. In each calculation, 400 computational cells were used in a one meter long domain, the fluid interface is initially located at 0.5 m, the CFL number was 0.75, and the final output time was 200 μs. The initial temperature of the gas was 300 K and the specific heat ratio was 1.667. The
parameters for the Tait fluid were $\rho_{ref} = 1000 \text{ kg/m}^3$, $N = 7.15$, $A = 1 \text{ bar}$, and $B = 3310 \text{ bar}$. Note that each of these calculations were actually performed in two dimensions on a planar slab, with the hyperbolic operator active in both directions. Each calculation was performed with the interface in both x- and y-directions with nearly identical results.

The first problem consists of a gas-liquid shock tube where the gas and liquid are initially stationary. The gas is initially at a pressure of 1 bar, but the liquid is in a highly pressurized state at a pressure of 1000 bar. This sends a weak shock wave into the gas and a very strong rarefaction wave into the liquid. A comparison of the calculated and exact solution is shown in Figure 4.15 and the calculated and exact solutions compare very well with each other.

The next problem is identical to the previous problem, with the exception that the gas is initially pressurized to 1000 bar and the liquid pressure is 1 bar. In this case a very strong
shock wave is sent into the liquid and a relatively weak rarefaction wave propagates into the gas. The calculated and exact solutions, shown in Figure 4.17, agree very well.

To test the phase change capabilities of the interfacial Riemann solver, a case was setup where the liquid and the gas were initially at a pressure of 1 bar and stationary, but a velocity jump condition of \( [u] = 10 \text{ m/s} \) was impulsively applied at the interface. The sudden action of the blowing velocity sends a weak shock wave into the gas, raising the pressure slightly. Mechanical equilibrium must be maintained at the interface, thus a shock wave is also sent
into the liquid. Again, the exact and calculated solutions, shown in Figure 4.18, agree well. Only a slight bump in the liquid pressure is observed at $x = 0.2$ m.

The final verification test examines the capabilities of the interfacial Riemann solver for situations where pressure jumps resulting from surface tension and/or recoil effects from phase change are considered. As with the previous test, the gas and liquid were initially stationary and at a pressure of 1 bar. At $t = 0$, a pressure jump of $[p] = -10$ kPa is applied at the surface. This raises the liquid pressure and sends a shock wave into the liquid. Since a small negative velocity is induced in the liquid a very weak rarefaction wave is sent into the gas, which lowers the pressure of the gas phase near the interface. The condition of pressure is a jump across the interface which slightly reduces the liquid pressure (i.e., $p_{\text{liq}} < p_{\text{init}} - [p]$). The results from this computation, shown in Figure 4.19, compares very well with the exact solution. A very small oscillation of velocity (on the order of 1 mm/s) on the gas phase side is observed. When the gas-phase velocities are very low, the low Mach number adjustment procedure almost perfectly centers the interpolated velocities and significantly reduces any dissipation that damp out these small oscillations. These oscillations are extremely low and will not likely become harmful or even become noticeable in practical calculations.
Figure 4.19: Gas water shock tube with gas and water initially at 1 bar with a pressure jump of \([p] = -10\) kPa at time of 0.2 ms.

4.9.5 Ghost Cell Filling for the Parabolic Operator

The ghost cells for the parabolic operator are filled in a similar procedure to the hyperbolic operator. However, rather than filling guard cells fluxes at the cell edges are computed directly from the jump conditions presented in Chapter 2. The jump conditions on the stresses, heat flux, and mass diffusion fluxes are rotated from the normal direction to the direction of the cell face. The stresses normal and tangential to the interface are related to the stresses in the \(x\)- and \(y\)-directions by:

\[
\sigma_{nn} = \sigma_{xx}\hat{n}_x^2 + \sigma_{yy}\hat{n}_y^2 + 2\sigma_{xy}\hat{n}_x\hat{n}_y, \quad (4.64)
\]

\[
\sigma_{nt} = \sigma_{xy}(\hat{n}_x^2 - \hat{n}_y^2) + (\sigma_{yy} - \sigma_{xx})\hat{n}_x\hat{n}_y. \quad (4.65)
\]

Note that there is no condition on the normal stress tangential to the interface, \(\sigma_{tt}\). Thus, when rotated to \(x\)- and \(y\)-directions there is generally a non-zero jump in \(\sigma_{xx}, \sigma_{yy}\), and \(\sigma_{xy}\) even when the jumps in the interfacial normal and shear stress are zero.
In terms of velocity gradients in the x- and y-directions, the jump in the normal stress is:

\[ [\sigma_{nn}] = \left( 2\mu_g \hat{n}^2_x + \mu'_g \right) \left. \frac{\partial u}{\partial x} \right|_g - \left( 2\mu_l \hat{n}^2_x + \mu'_l \right) \left. \frac{\partial u}{\partial x} \right|_l + \]
\[ \left( 2\mu_g \hat{n}^2_y + \mu'_g \right) \left. \frac{\partial v}{\partial y} \right|_g - \left( 2\mu_l \hat{n}^2_y + \mu'_l \right) \left. \frac{\partial v}{\partial y} \right|_l + \]
\[ 2\hat{n}_x\hat{n}_y \left( \mu_g \left. \frac{\partial u}{\partial y} \right|_g + \mu_l \left. \frac{\partial u}{\partial y} \right|_l - \mu_l \left. \frac{\partial v}{\partial x} \right|_l \right) + \]
\[ \eta \left[ \mu'_g v^g - \mu'_l v^l \right], \]

and the jump in the surface shear stress is:

\[ [\sigma_{nt}] = \mu_g \left( \hat{n}^2_x - \hat{n}^2_y \right) \left[ \left. \frac{\partial u}{\partial y} \right|_g + \left. \frac{\partial v}{\partial x} \right|_g \right] - \mu_l \left( \hat{n}^2_x - \hat{n}^2_y \right) \left[ \left. \frac{\partial v}{\partial y} \right|_l - \left. \frac{\partial u}{\partial x} \right|_l \right], \]

where \( \mu' = \kappa - 2/3\mu \) and \( u^g, u^l, v^g, \) and \( v^l \) are the gas and liquid velocities at the surface. Rotating the velocity jumps from the surface normal to the direction of the cell face gives:

\[ u^g - u^l = \hat{n}_x[u_n] - \hat{n}_y[u_t], \]
\[ v^g - v^l = \hat{n}_y[u_n] + \hat{n}_x[u_t]. \]
Discretization of the stress and velocity conditions depends on whether they are to be applied on an face in the x- or y-directions and on the sign of the surface normal vector. Consider the case, shown in Figure 4.20, where the stress jump condition is to be applied on a x-face and the normal vector is pointing to the right. The normal and shear stress jump conditions are:

\[
[\sigma_{nn}] = \text{sgn}(\hat{n}_x)[2\mu_g\hat{n}_x^2 + \mu'_g]\frac{u^g_r - u^g_l}{\Delta x} - \text{sgn}(\hat{n}_x)[2\mu_l\hat{n}_x^2 + \mu'_l]\frac{u^l_r - u^l_g}{\Delta x} + \\
2\text{sgn}(\hat{n}_x)\hat{n}_x\hat{n}_y\mu_g\frac{v^g_r - v^g_l}{\Delta x} - 2\text{sgn}(\hat{n}_x)\hat{n}_y\mu_l\frac{v^l_r - v^l_g}{\Delta x} + \\
2\hat{n}_x\hat{n}_y\mu_g\frac{\partial u}{\partial y}|_g - 2\hat{n}_x\hat{n}_y\mu_l\frac{\partial u}{\partial y}|_l + [2\mu_g\hat{n}_y + \mu'_g]\frac{\partial v}{\partial y}|_g - [2\mu_l\hat{n}_y + \mu'_l]\frac{\partial v}{\partial y}|_l + \\
\frac{\eta}{y}\left[\mu_g\frac{v^g_r + v^g_l}{2} - \mu_l\frac{v^l_g + v^l_r}{2}\right],
\]

and

\[
[\sigma_{nt}] = \mu_g(\hat{n}_x^2 - \hat{n}_y^2)\left[\frac{\partial u}{\partial y}|_g + \text{sgn}(\hat{n}_x)\frac{v^g_r - v^g_l}{\Delta x}\right] + 2\mu_g\hat{n}_x\hat{n}_y\left[\text{sgn}(\hat{n}_x)\frac{u^g_r - u^g_l}{\Delta x} - \frac{\partial v}{\partial y}|_g\right] - \\
\mu_l(\hat{n}_x^2 - \hat{n}_y^2)\left[\frac{\partial u}{\partial y}|_l + \text{sgn}(\hat{n}_x)\frac{v^l_r - v^l_l}{\Delta x}\right] + 2\mu_l\hat{n}_x\hat{n}_y\left[\text{sgn}(\hat{n}_x)\frac{u^l_r - u^l_g}{\Delta x} - \frac{\partial v}{\partial y}|_l\right],
\]

where \(u^g_r, u^g_l, u^l_r\) and \(u^l_g\) refer to the real and ghost x-velocity for the gas and liquid cells. The \(\text{sgn}(\hat{n}_x)\) term accounts for the fact that the the real and ghost cells switch spatial positions if the gas is on the left and the liquid is on the right. The velocity jump conditions are discretized by:

\[
\frac{u^g_r - u^g_l}{2} = \hat{n}_x[u_n] - \hat{n}_y[u_t] + \frac{u^l_r - u^l_g}{2}, \tag{4.72}
\]

\[
\frac{v^g_r - v^g_l}{2} = \hat{n}_y[u_n] + \hat{n}_x[u_t] + \frac{v^l_r - v^l_g}{2}. \tag{4.73}
\]

Before these above four equations can be applied, y-derivatives need to be determined and the jump conditions need to be determined. Gradients in the y-direction are approximated
using data from the real cells:

\[
\left. \frac{\partial u}{\partial y} \right|_g \approx \begin{cases} 
\frac{u_{i+1,j+1}-u_{i+1,j-1}}{2\Delta y} & \text{if } \phi_{i+1,j+1} \text{ and } \phi_{i+1,j-1} \geq 0 \\
\frac{u_{i+1,j+1}-u_{i+1,j}}{\Delta y} & \text{if } \phi_{i+1,j+1} \geq 0 \\
\frac{u_{i+1,j}-u_{i+1,j-1}}{\Delta y} & \text{if } \phi_{i+1,j-1} \geq 0 \\
0 & \text{otherwise}.
\end{cases}
\] (4.74)

This procedure is repeated for \( u, v, T, u_t \), and the calculation of the species mass diffusion fluxes. Determination of velocity and temperature partial slip conditions requires gradients of tangential velocity and temperature in the normal direction. Thus, approximation of gradients in the x-direction prior to the evaluation of the jump conditions are needed. These are estimated using first-order finite differences:

\[
\left. \frac{\partial T}{\partial x} \right|_g \approx \begin{cases} 
\frac{T_{i+2,j}-T_{i+1,j}}{\Delta x} & \text{if } \phi_{i+2,j} \geq 0 \\
0 & \text{otherwise},
\end{cases}
\] (4.75)

and is similar for the species mass diffusion fluxes and tangential velocity. The estimated temperature, diffusion fluxes, and tangential velocity gradients are rotated to the surface normal and tangential directions. Finally, the ghost velocities and ultimately the deviatoric stresses can be completed by solving the four discretized jump conditions simultaneously.

The species mass diffusion flux boundary conditions are far more direct:

\[
J''_x = \hat{n}_x J''_n - \hat{n}_y J''_t, \\
J''_y = \hat{n}_y J''_n + \hat{n}_x J''_t,
\] (4.76) (4.77)

where \( J''_n \) is determined from the boundary condition, Eq. (2.80) and \( J''_t \) is estimated using the mole fraction gradient in the tangential direction.

The temperature jump condition is:

\[
\frac{T_g^g - T_g^l}{2} = \frac{T_r^l - T_r^g}{2} + [T]
\] (4.78)
and the energy balance at the interface, Eq. (2.85), is approximated as:

\[
\frac{\lambda_g T^g_g + \lambda_l T^l_g}{\Delta x} = \frac{\lambda_g T^g_r + \lambda_l T^l_r}{\Delta x} + \rho_r r_p \left[ h^l_r - h^g_r - \frac{|v_r|^2}{2} \right] + \frac{1}{2} \sigma_{xx,g} (u^g_r + u^g_g) + \frac{1}{2} \sigma_{xy,g} (v^g_r + v^g_g) - \sum_i N_s J''_{i,n} h_i,
\]

(giving two equations and two variables for the liquid and gas ghost temperatures. Note that the viscous dissipation is not added to the liquid phase portion of the jump condition since it is not modeled in the liquid energy equation. Once the ghost temperatures are determined, the net heat flux at the gas and liquid sides of the surface are:

\[
q''_{x,g} = -\text{sgn}(\hat{n}_x)\hat{n}_x \frac{T^g_g - T^g_r}{\Delta x} - \hat{n}_y \lambda_g \frac{\partial T}{\partial y} \bigg|_g + \sum_i N_s J''_{i,n} h_i - \frac{1}{2} \sigma_{xx,g} (u^g_r + u^g_g) + \frac{1}{2} \sigma_{xy,g} (v^g_r + v^g_g),
\]

and

\[
q''_{x,l} = -\text{sgn}(\hat{n}_x)\hat{n}_x \frac{T^l_g - T^l_r}{\Delta x} - \hat{n}_y \lambda_l \frac{\partial T}{\partial y} \bigg|_l.
\]

The procedure for the stresses and diffusion fluxes on the y-faces is similar and not presented for the sake of brevity.

It was discovered that rotating the stress tensor was unstable on fine meshes. Leaving the velocity jump conditions, diffusion fluxes, and heat fluxes in the rotated state but assuming the stresses were in the x- and y-directions (i.e., \(\hat{n}_x = \text{sgn} \hat{n}_x\) in the stress jump conditions) did not lead to instability when two RKC stages were added in an ad-hoc manner. In the future it would be useful to derive a stability criterion for the surface stress condition.

Unlike the interfacial hyperbolic operator, there are not many exact solutions that can be exploited to verify the parabolic operator. Test problems such as Poiseuille in a partially filled gas-liquid tube or Hill’s spherical vortex take a very long time to establish steady state since the time-step size is governed by the liquid sound speed. In place of these tests, phenomena such as the separation angle of flow over a sphere and comparing the rate of heat flux from a sphere to the value estimated from a Nusselt correlation are examined in Chapter 5.
One practical verification is testing heat conduction from a heated planar liquid surface to a gas layer, which has the exact solution from two semi-infinite bodies in contact if the hyperbolic operator is not advanced and the properties are frozen. A gas-liquid interface was placed at \( x = 0.51 \) m in a one meter domain, discretized with 400 cells. The solution was marched in time using RKC with 2 stages for 200 s. Two cases were considered; case A with \( \rho_l = 1000 \text{ kg/m}^3, C_p_l = 4184 \text{ J/kg}, \) and \( \lambda_l = 0.6 \text{ W/mK} \) and case B with \( \rho_l = 10 \text{ kg/m}^3, C_p_l = 418.4 \text{ J/kg}, \) and \( \lambda_l = 0.006 \text{ W/mK} \). In both cases the gas was pure argon at atmospheric pressure and a temperature of 300 K with the thermal conductivity fixed at \( \lambda_g = 0.016 \text{ W/mK} \). A comparison of the exact and calculated solutions is shown in Figure 4.21, where the green line representing the computed solutions is on top of the exact solution.

4.10 Updating Conserved Variables

Most calculations using the level set method, such as the method of Nourgaliev et al. [44], advance the hyperbolic terms and the level set equation together. This practice leads to a complex algorithm when a computational cell changes its sign during the middle of a time step. To greatly simplify the scheme, the level set equation is frozen for the entire hydrodynamic time step including both hyperbolic steps, both parabolic steps, and
the source term step. After the fluid Navier-Stokes equations have been fully advanced, the
level set equation is advanced for a time-step of $2\Delta t$.

After the level set equation is advanced in time, the sign of $\phi$ may change in some
computational cells, (i.e., $\phi_{i,j}^{n+2}\phi_{i,j}^n < 0$), which need to be initialized. One common approach
is to extrapolate the conserved variables from the normal direction or use the solution from
the interfacial Riemann problem to initialize these cells. In this work these cells are filled
directly from the upwind cell. Once a cell that changes its sign is identified, the local interface
velocity, $v_{\text{loc}} = v_l - n_b \hat{n}$, is identified. A weighting function is then calculated at all four
surrounding cells:

\begin{align*}
W_1 &= \max(u_{\text{loc}}, 0) \max(0, \text{sgn}(\phi_{i-1,j}^n)), \\
W_2 &= \max(-u_{\text{loc}}, 0) \max(0, \text{sgn}(\phi_{i+1,j}^n)), \\
W_3 &= \max(v_{\text{loc}}, 0) \max(0, \text{sgn}(\phi_{i,j-1}^n)), \\
W_4 &= \max(-v_{\text{loc}}, 0) \max(0, \text{sgn}(\phi_{i,j+1}^n)).
\end{align*}

The cell is initialized directly from the neighboring computational cell that has the highest
value in the weighting vector.
RESULTS AND DISCUSSION

5.1 Gas Phase Validation Test Problems

5.1.1 Advection of a Gaseous Bubble

This problem tests the advection of a high-temperature helium bubble in nitrogen carrier gas. The temperature of the helium is 2000 K and the temperature of the nitrogen is 1000 K. The velocity of the carrier gas and bubble were 100 m/s and the calculation ended when the bubble traversed a distance of 1 m. The solution was advanced in time using the double-flux model of Billet and Abgrall [77] with fifth-order WENO-SymBO to interpolate the primitive variables. Sixty cells were placed in the helium bubble and the CFL number was fixed at 0.3. A comparison between the calculated and exact solution and the conservation errors are shown in Figure 5.1. The comparison between the calculated and exact temperature profiles is quite good with relatively limited dissipation, considering the coarseness of the grid. The double-flux model perfectly preserves the pressure, without any fluctuations, at the cost of introducing conservation errors. The conservation errors are negligible for mass and momentum, while the conservation error for the energy is around 0.48% at the end of the calculation. The higher conservation error in energy is primarily caused by artificial dissipation mixing chemical species while holding $\rho h_0^m$ constant. These minor conservation errors have to be tolerated since advection problems cannot be calculated using standard conservative methods (as demonstrated in Figure 3.4).
Figure 5.1: One-dimensional helium bubble advection test: (a) calculated temperature and pressure profiles after a traversal of 1 m and (b) conservation errors as a function of time.

5.1.2 Multi-component Shock Tube Problem

This test problem calculates a Riemann problem in a one meter-long tube with initial conditions given by:

\[
\begin{align*}
    T_L &= 300 \text{ K} & T_R &= 300 \text{ K} \\
    u_L &= 0 \text{ m/s} & u_R &= 0 \text{ m/s} \\
    p_L &= 10 \text{ atm} & p_R &= 1 \text{ atm} \\
    Y_{\text{He},L} &= 1 & Y_{\text{He},R} &= 0 \\
    Y_{\text{N}_2,L} &= 0 & Y_{\text{N}_2,R} &= 1,
\end{align*}
\]

with the discontinuity placed at \( x = 0.4 \text{ m} \). The solution was marched in time using RK3 with a CFL number of 0.3, 1000 cells in the domain, and fifth-order WENO-SymBO for characteristic variable interpolation. The solution and conservation error at a time of 300 \( \mu \text{s} \) are shown in Figure 5.2.

An exact solution for comparing with the calculated results does not exist since the mixture specific heat ratio is a function of species composition and temperature. Fortunately, the procedure outlined in John [183] can be used to calculate properties of the post-shock state and shock-wave velocity. A comparison of the calculated and the exact shocked state are shown in Table 5.1. The differences between the calculated and the exact shocked states
Figure 5.2: Helium/nitrogen shock tube test; (a) calculated pressure, density, and mass fraction profiles at 300 µs and (b) conservation errors as a function of time.

Table 5.1: Comparison between estimated and calculated shocked state for the He/N\textsubscript{2} shock tube problem.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Calculated</th>
<th>Exact</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{\text{shock}}$ (m/s)</td>
<td>709.2</td>
<td>712.0</td>
<td>0.39</td>
</tr>
<tr>
<td>$P$ (MPa)</td>
<td>0.4610</td>
<td>0.4617</td>
<td>0.15</td>
</tr>
<tr>
<td>$\rho$ (kg/m\textsuperscript{3})</td>
<td>3.06</td>
<td>3.03</td>
<td>0.33</td>
</tr>
<tr>
<td>$T$ (K)</td>
<td>507.1</td>
<td>513.1</td>
<td>1.16</td>
</tr>
<tr>
<td>$u$ (m/s)</td>
<td>445.7</td>
<td>444.7</td>
<td>0.22</td>
</tr>
</tbody>
</table>

are quite small, slightly greater than 1% in the worst case for the post-shock temperature, and can be tolerated. Despite the conservation errors, the Riemann problem is calculated with a high degree of accuracy.

5.1.3 Laminar Premixed Flame

This problem consists of calculating the speed that a planar flame propagates into a fuel/air mixture. The initial conditions in most of the domain contained a stoichiometric mixture of air and ultrafine liquid aluminum particles at a temperature of 300 K, atmospheric pressure, and zero velocity. A very small portion at the left side of the domain was initialized
at the equilibrium flame condition to serve as an ignition source. Initially, diffusion transports heat and intermediate chemical species to the unburned reactants. Shortly afterwards, chemical reactions occur that convert chemical energy into sensible energy and sustain large temperature and mass fraction gradients between products and the reactants. Eventually, a steadily propagating flame is produced. This test is a very challenging test for an unsteady, compressible, reacting flow code due to the very low Mach number condition (at most on the order of 0.05) and the delicate interplay between convection, nonlinear diffusion, and chemical reactions that must be calculated properly.

The one-dimensional Navier-Stokes equations were integrated using fifth-order WENO-SymBO to interpolate the primitive variables with an overall time step determined by a CFL number of 0.3. The cell spacing was 2.5 µm, and diffusion processes were calculated using both Runge-Kutta-Chebyshev (RKC) and sub-cycling the first-order Euler method five times. Computed results using RKC and sub-cycling Euler’s method were nearly identical and a comparison is not shown. The left boundary condition was treated using an outlet condition with a specified pressure of one atm. A non-reflecting condition [152] was used as the right boundary condition. The inhomogeneous terms due to chemical reactions were calculated using the gaseous Al/O reaction mechanism of Huang et al. [11], which consisted of 11 species and 12 reactions and given in Table 2.1 with the addition of the following two reactions:

\[ \text{Al} \rightleftharpoons \text{Al}(l) \]  \hspace{1cm} (5.2)  \\
\[ \text{Al}_2\text{O}_3 \rightleftharpoons \text{Al}_2\text{O}_3(l) \]  \hspace{1cm} (5.3)

where \( A = 1 \times 10^{14} \text{ s}^{-1} \), \( n = 0 \), and \( E_a = 0 \) for both condensation reactions.

Exact solutions to this problem are impossible due to its nonlinearity. In place of an exact solution, the calculated results from this work were compared to those using Chemkin 4.1.1 [184] and are shown in Figure 5.3. The calculated results from this work agree very well with Chemkin solution. The laminar flame speeds, \( S_L \), differ by only 1.12%. The calculated temperature and species profiles are also in excellent agreement with very minor differences.

### 5.1.4 One-Dimensional H\(_2\)/O\(_2\)/Ar Detonation

In this problem the diluted H\(_2\)/O\(_2\)/Ar Chapman-Jouget (CJ) detonation wave with molar ratios of 2:1:7 at an initial pressure and temperature of 6.67 kPa and 298 K, respectively,
Figure 5.3: Comparison between computed laminar premixed flame structures using the numerical methods developed in this thesis and Chemkin 4.1.1: (a) temperature and flame speed and (b) species mole fractions.

is simulated. Oran et al. [185] and Deiterding [186] studied this problem extensively using both reduced and complex chemical reaction mechanisms. The reaction mechanism used in this work consisted of 9 species (H$_2$, O$_2$, Ar, OH, H$_2$O, HO$_2$, H$_2$O$_2$, H, and O) and 34 irreversible reactions [187].

The detonation was initiated by propagating a shock wave, initially placed at $x = 3$ cm, with a velocity of 1650 m/s into the unreacted mixture. The initial shock wave is strong enough to ignite the mixture in a reasonably short period of time, but not so strong that the resulting detonation wave is overdriven. The boundary conditions on the left side of the domain were perfectly reflecting and non-reflecting conditions were used on the right. The fifth-order hybrid method was used with $\Delta p_s = 1$ Pa and the LM adjustment. The AUSM dissipation parameters were changed to $K_p = 1$, $K_u = 1$, and $\sigma = 0.25$ when the characteristic variables were interpolated to suppress oscillations that could interfere with the speed and structure of the CJ detonation wave. The solution was marched in time using RK3 with a CFL number of 0.95 until the velocity of the detonation wave relative to the upstream gas velocity reached a steady value, as shown in Figure 5.4.

The structure of the calculated CJ detonation wave is shown in Figure 5.5, and agrees quite well with the reference calculations of Deiterding [186]. The small spike in the hydrogen mass fraction at the location of the leading shock ($x = 1.222$ m) is caused by baro-diffusion.
Figure 5.4: Convergence of the detonation wave velocity on the medium grid: (a) pressure profiles at various times and (b) location of the leading shock as a function of time.

Figure 5.5: Structure of the CJ detonation wave calculated using the fine grid at $t = 711 \mu s$: (a) temperature, pressure, density, and velocity profiles and (b) species mass fraction profiles.

The detonation velocity and structure were calculated using three grids with cell spacings of $\Delta x = 31.25 \ \mu m$, 62.5 $\mu m$, and 125 $\mu m$. A comparison between the calculated detonation velocity, $c_{det}$ and pressure in the von Neumann spike, $p_{vn}$, and temperature in the von Neumann spike, $T_{vn}$, are shown in Table 5.2. The temperature and pressure in the von Neumann spike differ from the reference calculation [186] by only 6.5 K and 3.4 kPa and
Table 5.2: Comparison of grid convergence on the calculated CJ detonation parameters.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Coarse</th>
<th>Medium</th>
<th>Fine</th>
<th>Reference [186]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{det}$ (m/s)</td>
<td>1616.0</td>
<td>1618.3</td>
<td>1619.8</td>
<td>1626.9</td>
</tr>
<tr>
<td>$p_{vn}$ (kPa)</td>
<td>174.1</td>
<td>172.7</td>
<td>173.9</td>
<td>177.3</td>
</tr>
<tr>
<td>$T_{vn}$ (K)</td>
<td>1910.0</td>
<td>1919.8</td>
<td>1915.2</td>
<td>1921.7</td>
</tr>
</tbody>
</table>

Figure 5.6: Initial and boundary conditions for the re-shocked Richtmyer-Meshkov instability.

there is only a difference of 7.1 m/s between the calculated detonation velocities using the finest mesh. It is also clear that the LM hybrid characteristic/primitive variable method performs quite well for either of the meshes used; calculations on the coarsest mesh are also very close to the reference calculation.

5.1.5 Re-shocked Richtmyer-Meshkov Instability

The re-shocked Richtmyer-Meshkov (RM) instability, initially simulated by Latini et al. [188], is where a Mach 1.21 shock wave in a mixture of air and acetone vapor interacts with a sinusoidal SF$_6$ interface. This was simulated using the fifth-order hybrid multi-component technique developed in this work. A schematic diagram of the initial conditions for this problem is shown in Figure 5.6. The interface is initially perturbed with a sinusoidal function $\eta(y) = a_0 \sin(2\pi y/\lambda)$ where the amplitude of the initial perturbation is 0.2 cm and the wavelength is 5.93 cm. To compare the results with those of Latini et al., the interface is smeared using Eq. (3.125) so that the interface is spread over a thickness of $\delta = 5$ mm. The initial pressure in the domain was set to 95.6 kPa and the initial temperature of the
The air/acetone mixture was 296 K. The Atwood number:

\[ At = \frac{\rho_{SF_6} - \rho_{air/acetone}}{\rho_{SF_6} + \rho_{air/acetone}} \],

was set to 0.6053 and used to calculate the initial temperature of the pre-shocked SF$_6$. The solution was marched in time using RK3 to integrate the hyperbolic terms and RKC to integrate the parabolic terms. The CFL number set to 0.5 and the hybrid fifth-order method with the LM adjustment to interpolate variables to the cell edges. The rotated Riemann solver was turned off by setting $\epsilon_{rot} = 1.5$, and $\Delta p_s$ was fixed at 100 Pa. AMR was used on 12×12 blocks with seven levels of refinement and a resolution of $\Delta x = 116 \, \mu m$ (512 cells per perturbation wavelength). The evolution of the acetone mass fraction is shown in Figure 5.7.

The shock wave in the air/acetone mixture interacts with the perturbed SF$_6$ interface, which produces vorticity at the interface due to misalignment of the pressure and density gradients. Two spikes form, grow, and eventually roll up. At around 6.6 ms the reflected shock wave interacts with the interface a second time, producing a complex and low Mach number flow field that transitions to turbulence. The low-dissipation hybrid fifth-order

\[ \text{Figure 5.7: Calculated mass fraction of acetone at various times indicating the evolution of the re-shocked Richtmyer-Meshkov instability with a grid resolution of } \Delta x = 116 \, \mu m. \]
method produces very fine flow-field structures which compare qualitatively well with the ninth-order results of Latini et al. [188].

The effect of low-Mach number adjustment, slope limiter, and grid resolution on the acetone concentration at a time of 16 ms is shown in Figure 5.8. It is clear that both the LM adjustment procedure and selective application of the slope limiter both increased resolution of the material interfaces and produce finer vortex structures. Applying the slope limiter everywhere, $\epsilon_s = 0$, without the low-Mach number adjustment produced the least resolved and largest vortices. The LM adjustment procedure drastically reduced dissipation and increases resolution of the flow-field structures, even though it was originally designed for use with the HLLC approximate Riemann solver. Selective application of the slope limiter, $\epsilon_s = 0.001$, also increased resolution of the material interface and produced finer structures in the acetone mass fraction field. A more detailed comparison requires the extraction of the turbulent spectra, which is beyond the scope of this thesis.

### 5.1.6 Shock-wave/H$_2$ Cylinder Interaction

The reacting hydrogen cylinder and shock-wave interaction problem computed by Billet et al. [79] was repeated, where a hydrogen cylinder with a radius of 2.8 mm is impacted by a Mach two shock wave in air. To shorten the domain, a stationary shock wave was initialized.
at $x = 7$ mm and the H$_2$ cylinder travels through the shock. The velocity, temperature, and pressure of the pre-shocked air and hydrogen bubble were 1240 m/s, 1000 K, and 1 atm, respectively. The velocity, temperature, and pressure of the post-shocked air were 435 m/s, 1566 K, and 4.46 atm, respectively. The mass fraction of air and H$_2$ were initialized according to Eq. (3.125) with $C_r = 33,000$ and a center location at $x = 4$ mm. The dimensions of the domain were 22.5 mm × 7.5 mm with symmetry boundary conditions applied on the top and bottom and non-reflecting conditions applied on the left and right. The initial bubble position and shock-wave location are shown in Figure 5.9. Adaptive mesh refinement was used with 6 levels of refinement and each block containing an 18×18 grid, providing a computational cell size of $\Delta x = 13 \mu m$ at the finest level of refinement. A CFL number of 0.75 was used with RK3 to integrate the parabolic terms. RKC was used to integrate the parabolic terms with the criterion of Eqs. (3.84) and (3.85) producing, on average, four stages. The hybrid fifth-order method was used for spatial discretization with $\Delta p_s = 1$ atm and $\epsilon_{rot} = 0.5$. The reaction mechanism of the H$_2$/O$_2$ system consisted of 9 species and 19 reversible chemical reactions [189].

The temporal development of the H$_2$ bubble is shown in Figure 5.10 and is plotted in a similar manner to the format used by Billet et al. [79] for direct comparison. Contour plots of other variables at a time of 13.6 $\mu s$ is shown in Figure 5.11. The calculated results of this work compare very well with those of Billet et al. [79]. The evolution of the H$_2$ bubble and development of the pressure field are very similar; however, there are some differences, such as higher temperatures and different vortical structures. The low-dissipation method and finer grid used in this work provides a high quality solution with increased resolution of fluid instabilities. A simplified mixture-averaged diffusion flux formulation is used in this work,
Figure 5.10: Contours of hydrogen mass fraction (colored flood) and pressure (lines) with 100 contour lines between 1 and 8 bar showing the evolution of the hydrogen bubble and the development of the main vortex. Hydrogen mass fractions below 0.05 are not shown.
Figure 5.11: Computed results of the shocked H$_2$ cylinder at a time of 13.6 $\mu$s showing the density, temperature, Schlieren, and mass fractions of O$_2$, H$_2$O, and H$_2$O$_2$ fields.

while Billet et al. [79] used a more complete multi-component formulation. The differences in the diffusion flux formulation can lead to different rates of diffusion and explains why the hydrogen filament disappears near the main vortex at 8.8 $\mu$s in the present calculations, while the reference calculations do not show this disappearance even though Billet et al. [79] used a third-order method with higher dissipation. Another possible reason for these slight differences can be attributed to differences in the integration of the chemical source terms between this work and Billet et al. [79], who did not use a stiff chemistry solver but instead used a one-step scheme that limited the global time-step size based on the the hyperbolic, parabolic, and source term operators.

The effect of the global time-step size is shown in Figure 5.12. Calculations where the time-step size was fixed at $\Delta t = 10^{-10}$ s ($\text{CFL} \approx 0.05$) produced slightly better resolution of secondary vortices, but is otherwise very close to the case where the CFL number was fixed at 0.75.
Figure 5.12: Contours of hydrogen mass fraction at a time of 8.8 µs with different time-step sizes with a cell size of $\Delta x = 13 \, \mu m$.

Figure 5.13: Contours of hydrogen mass fraction at a time of 13.6 µs at different grid resolutions with CFL = 0.75.

The effect of grid resolution on the hydrogen mass fraction at a time of 13.6 µs is shown in Figure 5.13. Since this test involves fluid instabilities, grid convergence is impossible until the size of the computational cells is significantly smaller than the Kolmogorov scale (about 2.5 µm), which is impractical to achieve, even with AMR.

5.1.7 Viscous Two-Dimensional H$_2$/O$_2$/Ar Detonation

In this numerical experiment the multi-dimensional detonation problem studied by Oran et al. [185] and Deiterding [186] is calculated to observe if the quasi-conservative method used
in this paper is capable of producing cellular detonation structures and forming additional triple points. The results from the 1-D CJ detonation calculation shown earlier are initialized on a two-dimensional domain measuring 30 cm $\times$ 3 cm, with the leading shock placed at $x = 3$ cm. To shorten the required length of the domain, the velocity field is altered so that the velocity upstream of the detonation is at $u = -c_{det}$. Non-reflecting boundary conditions were used at the left and right sides of the domain and symmetry conditions were enforced on the top and bottom. AMR was used with seven refinement levels on 14$\times$14 blocks, producing a computational cell size of $\Delta x = 33.5 \, \mu m$ at the finest level. The rotated Riemann solver was activated to suppress shock anomalies that may artificially alter the structure of the detonation with $\epsilon_{rot} = 0.5$. $\Delta p_s$ was set to 100 Pa. The hyperbolic terms were marched in time using RK3 with a CFL number of 0.95, and the parabolic terms were integrated using RKC with two stages. To reduce computational expense, the source term integrator was changed from VODE to CHEMEQ2 [190] with five correction stages and an error tolerance of $10^{-6}$.

Multi-dimensional detonations have physical instabilities that produce transverse shock waves and cellular structures. A small box of unreacted gas at a pressure of 47 kPa and a temperature of 2084 K with dimensions of 10 mm $\times$ 7 mm was placed at 3 mm behind the leading shock to perturb the 1-D detonation and allow the transverse instabilities to develop. Eventually a regular oscillating detonation structure, shown in Figure 5.14, involving a complex series of triple point collisions and transverse shock waves form.

The computed results of this work, shown in Figs. 5.14 and 5.15, compare very well with those of Dieterding [186] and shows two triple points acting on the incident shock wave. Each triple point has a complex double Mach-reflection structure [191], which is well captured by the present numerical method. The effect of grid resolution on the double Mach-reflection structure is shown in Figure 5.16. At low grid resolution, the grid size is too large to resolve the details of the triple point structure and the double Mach-reflection structure disappears. Even though the details of the double Mach-reflection disappear with the coarse grid, the overall structure detonation wave was relatively unchanged.
5.2 Multiphase Calculations

5.2.1 Dust-Gas Shock Tube Problem

There are not any exact solutions to non-trivial dusty gas problems, but the dust/gas shock tube problem has been calculated in Miura [192] and can be compared to qualitatively. In this problem the domain was one cm long and a diaphragm separating high-pressure pure gas on the left and a dust-gas mixture on the right was located at \( x = 3.75 \) mm and was discretized with 400 computational cells. The pressure of the left state was 10 atm and the pressure of the right state was at atmospheric pressure. The initial temperature and velocity
of both states was 1000 K and 0 m/s, respectively. In all computations the volume fraction of the alumina particles was $3 \times 10^{-5}$, but three different particle diameters were considered: 0.01, 0.1, and 1 $\mu$m. The solution was marched to a time of $t = 4 \mu$s using RK2 with a CFL number of 0.5.

The computed results from the dust-gas shock tube problem are shown in Figure 5.17. The solution compares well with the results of Miura [192]. The particles, which were initially motionless, are accelerated by drag from the post-shock gas. The increase of momentum to the condensed phase is matched by a decrease in momentum to the gas phase. The decrease in gas-phase velocity increases the pressure. Even though the gas phase pressure is higher in the dusty cases, the strength and velocity of the shock wave is lower than the pure-gas cases. The smaller-diameter particles mechanically and thermally equilibrate almost immediately behind the shock wave. The largest not had enough time to equilibrate and do not have enough time to closely follow the gas-phase temperature and velocity.

5.2.2 Shock and Dust Layer Interaction

An extreme example of how the presence of dust can influence the propagation of a shock wave is the shock wave and dust layer interaction problem. The initial conditions are shown in Figure 5.18. A Mach two shock wave is initialized in stagnant air at atmospheric pressure and a temperature of 300 K. The particles were taken to be alumina at a temperature of 300 K with a diameter of 100 nm. To exaggerate the influence of the dust layer on the shock
Figure 5.17: Computed results of the alumina dust-gas shock tube problem at a time of $t = 4 \mu s$. 
Figure 5.18: Initial conditions for the shock wave and dust layer interaction problem.

wave, the volume fraction of the dust layer was very high at $\alpha = 0.001$. The hyperbolic terms were directionally split and marched in time with a CFL number of 0.5 using RK2. RKC was used to integrate the parabolic terms with two stages. AMR was used with five levels of refinement on $20 \times 20$ cell blocks.

The evolution of the computed Schlieren and dust volume fraction is shown in Figure 5.19. Unlike the dust-gas shock tube problem, the high volume fraction affects the propagation of the shock wave substantially. At around $2 \, \mu s$ the incident shock wave impacts the dust layer and a fairly strong shock wave is reflected and the transmitted shock in the dust layer slows tremendously. The complex reflection produces a region of very high vorticity on the top-left corner of the dust pile, which entrains the left edge of the dust layer. As the incident shock wave travels further, the transmitted shock wave becomes more and more oblique, dragging some of the particles towards the centerline and compressing the dust pile. At later times Kelvin-Helmholtz instabilities form on the top of dust layer and on the edge of the main vortex. The computed results in this work compare fairly well with the shock wave and dust layer interaction problems computed by Collins et al. [144], where a much more dissipative scheme was used for the gas phase. They computed similar results, but had much less resolution of the Kelvin-Helmholtz instabilities and the main vortex.

5.2.3 Multiphase Adiabatic Constant-Volume Reactor

A stoichiometric mixture of liquid Al and air was placed in a closed and adiabatic constant volume reactor and then integrated in time. The initial conditions of the stoichiometric mixture of liquid aluminum and air was atmospheric pressure and a temperature of 2700 K. Three alumina condensation models were considered: homogeneous, continuum, and Dahneke. The gas-phase reaction mechanism is taken from Huang et al. [11] and is given in Table 2.1. The homogeneous condensation model treats the liquid alumina as a gas-phase species and calculates the rate of condensation using a very fast reversible chemical reaction between gaseous and liquid alumina [11]. The continuum and Dahneke condensation models
both treat the condensed phase alumina droplets as a multiphase mixture. Their difference lies in that the condensation rate in the continuum model does not take into account the correction for high Knudsen numbers [see Eq. (2.36)], while the Dahneke version does.

The constant volume reactor was marched in time using DVODE with the error tolerance set to $10^{-8}$. A comparison of the three different models is shown in Figures 5.20 through 5.22. The computed final equilibrium temperature is very close among all three models, with a very slight lowering of temperature (see Figure 5.21a) when either the continuum or Dahneke multiphase condensation models are used. This is due to the difference in how alumina is treated between the homogeneous and multiphase models. The homogeneous model treats alumina an ideal gas with the specific energy of condensed-phase alumina, while the multiphase models treat the alumina as heavy condensed-phase particles. When mass exchanges from the gas to the condensed phase, the overall gas density decreases and along with it the pressure, as shown in Figure 5.21b. Since the equilibrium flame temperature of alumina/air is a function of pressure, the decrease in pressure also decreases the flame temperature. Of all three models the homogeneous condensation model reacts the fastest with the entire event taking less than one microsecond. Accounting for nucleation prolongs
Figure 5.20: Comparison of the computed species mass fractions in a constant volume reactor using three different alumina condensation models.

the reaction time substantially to around 3 $\mu$s for the continuum and 90 $\mu$s for the Dahneke model.

The primary difference between the two multiphase models is the rate of nucleation, the equilibrium particle number density, and the equilibrium volume-averaged diameter, shown in Figure 5.22. The Dahneke model accounts for high Knudsen number effects, while the continuum model was derived by using the continuum approximation. The continuum assumption overestimates the condensation rate of the particles when they are very small. The condensation rate is more than four orders of magnitude greater than the nucleation rate for the continuum model, while the condensation rate for the Dahneke model is only around
two orders of magnitude larger. Thus, condensed-phase particles have a greater tendency to nucleate using the Dahnke model, while they have a greater tendency to grow with the continuum model. In either case the final volume fraction of the particles was $1.14 \times 10^{-5}$ and the diameter of the particles are nano-sized. The results from the dusty-gas shock tube problem shown above indicate that there is a noticeable, but relatively small effect on the propagation of a shock wave in a mixture of aluminum particles with a volume fraction of $3 \times 10^{-5}$ and a particle diameter of 10 nm.

It is anticipated that shock wave propagation through an alumina layer produced from a diffusion flame would have much less of an effect than shown above because the computed volume fraction of alumina in the constant volume reactor is roughly a third of the value used to compute the dust-gas shock tube problems. Since the volume-average particle diameter is on the order of 10 nm, it would be expected that the condensed-phase alumina droplets would almost instantly become flow-borne in the post-shock gases. Thus, treating the condensed-phase alumina as an ideal gas in the final calculations is likely acceptable. Treating alumina as an ideal gas also has the advantage of reducing the number of conservation equations by four and removes three sources of stiffness for the source term integrator: nucleation and condensation, particle drag, and particle heat transfer. Neglecting the dusty gas model will also avoid the small conservation error shown in Figure 5.22c.

Figure 5.21: Comparison of temperature and pressure in a constant volume reactor using three different alumina condensation models.
In the derivation of the RHS vector for the source term operator, terms involving $\rho_c \partial \alpha_c / \partial t$ in the gas-phase source terms were neglected, which introduces a slight conservation error of around $10^{-7}$. This error is associated with the model itself and cannot be corrected by adjusting the error tolerances of the ODE solver.
5.2.4 Interaction Between a Shock Wave and a Heated Aluminum Droplet

The interaction between a Mach four shock wave propagating into air at a pressure of one atmosphere and a temperature of 300 K and a 230 µm diameter aluminum droplet at 2750 K was calculated using five levels of refinement on 20×20 blocks with a resolution of approximately 256 cells across the droplet diameter. Axisymmetric coordinates were used with the x-axis serving as the axis of rotation. The air surrounding the droplet was initially at a temperature of 300 K and atmospheric pressure. The energy equation was solved in the liquid phase. The hyperbolic operator was directionally split with the CFL number fixed at 0.5 and integrated using RK2. The parabolic terms were integrated using RKC with four stages. Phase change was neglected, but surface tension and partial slip conditions were taken into account. The initial conditions are shown in Figure 5.23. A time sequence of the Schlieren and pressure evolution at early times is shown in Figure 5.24 and the evolution of the Schlieren and temperature fields at later times is shown in Figure 5.25.

Initially, the very sharp temperature gradient at the surface of the liquid Al droplet produces a high rate of heat conduction into the gas. As a result, the temperature of the gas near the droplet rises during the parabolic step. Since density is fixed during the parabolic step, pressure rises with temperature and a strong thermally induced acoustic wave is produced. After 20 ns have elapsed, the shock wave impacts the liquid droplet, which transmits a very weak shock wave into the droplet and reflects as a very strong shock wave in the gas. Due to the very high sound speed of liquid Al, the liquid shock wave travels much faster in the liquid, causing it to diffract and weaken. When the diffracted shock wave in the liquid interacts with the upper surface a rarefaction wave is reflected into the droplet producing a free von Neumann refraction. As the shock wave travels past the equator, the

![Figure 5.23: Initial conditions for the shock wave and heat droplet interaction problems.](image-url)
Figure 5.24: Early time sequence of the computed Schlieren and pressure fields of a Mach four shock wave interacting with a heated Al droplet at 2750 K. Pressures below 2 kPa are colored white.
so-called anomalous reflection is formed [193, 194]. As time continues the free von Neumann refraction strengthens and becomes strong enough to induce a cavitation bubble (indicated by the white region in the pressure fields in Figure 5.24) near the surface. After 84 ns, the shock wave reflects off rear surface of the droplet as a very strong rarefaction wave, producing a very large cavitation bubble. At later times the pressure in the droplet increases and the cavitation bubble collapses, producing a shock wave.
The process of cavitation bubble collapse is quite complex, as shown in Figure 5.26. After the initial cavitation bubble is formed the pressure in the droplet increases and the cavitation bubble collapses. As a cavitation bubble collapses a shock wave is formed in the liquid, which is shown by local increase in pressure near upper point of the cavitation bubble at $t = 133$ ns in Figure 5.26. This shock wave propagates outward from the collapsing cavitation bubble and reflects from the rear surface of the droplet as a rarefaction wave. Due to interactions from coalescing rarefaction waves, a second cavitation bubble forms at around $t = 140$ ns, which is closer to the rear surface of the droplet than the initial cavitation bubble. As time carries on, the overall pressure inside the droplet increases and the second cavitation bubble collapses. The collapse of the second cavitation bubble sends another shock wave and induces a third cavitation bubble very close to the droplet surface. After the third cavitation bubble collapses, the overall pressure in the droplet is high enough to inhibit the formation of any further cavitation bubbles.

Even though different liquid equations of state were different between this work and Nourgaliev et al. [44], the progression of the reflected and transmitted waves compare well. However, the diffracted shock wave in the gas-phase propagating around the droplet has a different structure than computed from an inviscid calculation. The difference is caused by conduction from the droplet increasing the temperature and sound speed of air near the droplet. This causes the shock wave to increase its speed locally near the droplet, giving it a more complex shape.

As time continues the reflected shock wave in the air turns into bow shock and pressure and drag forces deform the droplet. A wake, whose length is on the order of two droplet diameters, is formed. At 1.39 µs the rear side of the droplet flattens and deforms slightly. The slight deformation is initially started by locally high pressure caused by focusing of the diffracted shock wave on the rear of the droplet and continued by the strong recirculation zone. At around 2.09 µs a liquid filament is introduced by the Rayleigh-Taylor instability from the light gas pushing on the dense liquid. At later times the flattening of the droplet becomes more severe and the liquid filament continues to grow. The Weber number, $We$, is between 1200 and 2800 and $WeRe_d^{-1/2} \approx 8 - 15$, placing the droplet in the border between the flattening/stripping and shattering regimes. Since the Weber number is very low, it is expected that the droplet would be much more prone to flattening over stripping. Thus, the progression of the droplet shape shown in Figure 5.25 is in agreement with the droplet deformation and breakup criterion.
Figure 5.26: Cavitation bubble collapse and reformation sequence for a Mach four shock wave interacting with a heated Al droplet at 2750 K. Pressures below 2 kPa are colored white.

A time sequence of a Mach two shock wave interacting with an Al droplet is shown in Figure 5.27. The progression of the shock and transmitted wave is similar to the Mach four case, with the exception of the strength of the transmitted and reflected waves are much weaker and the region of cavitation is much smaller in size. The Weber number is on the order of 200 and \( WeRe_{d}^{-1/2} \approx 3 \), placing the droplet in the flattening/stripping regime, but much weaker than the Mach four case.
Figure 5.27: Time sequence of computed Schlieren and temperature fields for a Mach two shock wave interacting with a non-reacting heated 230 µm Al droplet.
Even though a cavitation bubble is formed inside the droplet for a brief period of time, it is not violent enough to induce spallation, which requires a very high initial pressure in the droplet. If the cavitation is very strong, the vacuum Riemann problem holds (see Chapter four of Toro [113] and the cavitating vacuum Riemann test problem in Section C.7); the spallation velocity is the tail speed of a cavitating rarefaction wave when the pressure of the starred state is zero:

\[ u_{\text{spall}} = -\int_{p_{\text{init}}}^{0} \frac{dp}{\rho c}, \] (5.5)

which has a magnitude on the order of 60 to 70 m/s if the initial pressure in the droplet is on the order of a few GPa. If the pressure of the liquid before cavitation is only around 0.001 GPa, the spallation velocity is much smaller, at most on the order of 0.1 m/s. Thus, to achieve spallation the initial pressure of the droplet must be very high and the pressure from the shock wave is not high enough.

The spallation velocities calculated using the vacuum Riemann problem for liquid Al are consistent with the melt dispersion mechanism of flame propagation of nano-Al particles [195, 196]. As stated in the introduction, the solid alumina shell surrounding the aluminum particle must be breached for the Al particle/droplet to ignite. While Al particles melt, the oxide layer cracks due to differences in expansion between solid alumina and melting aluminum. If the Al particle are nano-sized a tremendous amount of stress is needed to crack the oxide layer, resulting in liquid Al pressures up to 8 GPa. After the oxide shell is cracked, the surface of the molten Al is exposed to the much lower pressure gases, setting up a situation very close a spherical Riemann problem with pressurized liquid Al. Thus, rarefaction waves propagate into the droplet. Due to the focusing of the rarefaction waves that propagate into the liquid droplet a very strong cavitation bubble is formed in the center of the droplet. Since pressure in the droplet before cavitation occurs is high, the spallation velocity ranges from 50 to 250 m/s [195, 196], which is in the range of spallation velocities computed from the solution of the vacuum Riemann problem at high pressure conditions. The fragments of the spalled Al droplets race ahead of a propagating flame in suspensions of nano-sized Al particle and produce a significantly higher flame speed than predicted using diffusion-based mechanisms. For the melt dispersion mechanism to become active, the Al particle must be on the nano-scale. If the Al particles are micron sized, a much lower pressure on the order of 50 MPa is needed to crack the oxide shell [196] which results in significantly
reduced spallation velocities on the order 3 to 8 m/s, which is likely not enough to enhance the flame propagation velocity in a significant manner.

As a sanity test, the calculated total rate of heat loss from the droplet when is roughly spherical was compared to the correlated values for the total heat transfer over a sphere. Since the flow observed by the droplet is altered by a bow shock it is difficult to select a proper free stream value to apply a heat transfer correlation. Depending on what state and which heat transfer correlation is selected (e.g., Whitaker’s [197] or Carlson and Hoglund’s [99]), the Reynolds number over the particle for the Mach four case ranges from 25,000 to 35,000. The estimated rate of heat loss ranges from 7.7 to 10.7 W with a corresponding thermal time constant of 0.7 to 1.2 ms at $t = 0.7 \mu s$. At this time the calculated total rate of heat loss, shown in Figure 5.28a, is slightly lower at approximately 6.46 W. For the Mach two case, the Reynolds number is around 5,000 and the rate of heat loss is estimated to be between 3.2 and 3.7 W with a corresponding time constant of 1.7 ms at $t = 2 \mu s$.

It is not expected that the calculated heat transfer results would exactly match empirical estimations since heat transfer correlations over a sphere are intended for relatively steady state conditions and have a degree of uncertainty. The present calculation is not steady, highly compressible, and contains shock waves. Another item that lowers the heat loss rate from the droplet is significant viscous dissipation, especially with the Mach four case. Viscous dissipation converts kinetic energy to sensible energy in the boundary layer which reduces the temperature gradient near the droplet surface and ultimately the rate of heat loss. This effect accounted with heat transfer correlations over spheres.

The estimated thermal time constants are roughly 1000 times larger than the time scale of the calculation for either shock-wave strength. Thus, the sensible energy content of the liquid Al barely changes due to the short time scales of these computations. For the Mach four case at $t = 0.7 \mu s$, the liquid Al has reduced in temperature by only five Kelvin at the stagnation point and the thermal diffusion front has only propagated around 20 $\mu m$ into the droplet; the temperature elsewhere has not changed.

After about 1.5 $\mu s$ have elapsed in the Mach four case, the droplet deforms and the surface area, shown in Figure 5.28b, increases significantly. As a result the total rate of heat transfer increases along with the surface area.

An item that can be used to validate the viscous stress coupling algorithm is to compare the separation point when the droplet is roughly spherical. A contour plot of the velocity magnitude and streamlines at a time of 0.7 $\mu s$ is shown in Figure 5.29. The separation point
is approximately 21° behind the equator, which is fairly close to the experimental images from Chapter three of van Dyke [198]. The Reynolds number for the Mach two case is much lower and almost laminar, thus the separation point should be at, or immediately behind, the equator. The calculated streamlines for the Mach two case, shown in Figure 5.30, show that the flow separates at the equator.

Even though the Marangoni stress was included in these calculations, it turns out that it barely affects the computed results. Calculations with and without the Marangoni stress were nearly identical. The Marangoni number, $Ma$, is defined as:

$$ Ma = -\frac{d\sigma}{dT} \frac{lCp\Delta T}{\mu \lambda \rho} $$

where $l$ is a characteristic length. At $t = 1.39 \, \mu s$ the maximum and minimum temperature near the surface of the Al droplet are separated by $\Delta T = 6 \, K$. Taking the characteristic length to be the droplet radius and computing the thermal properties at $T = 2750 \, K$, the resulting Marangoni number is roughly 20. A Marangoni number this small is not high enough to induce significant convection inside and certainly not high enough to effect stability of the droplet surface which typically requires Marangoni numbers to be much greater than 1000 [199].
Figure 5.29: Comparison between (a) computed instantaneous streamlines showing the separation point at a time of 0.7 μs for the Mach four case and (b) experimental mean flow image at $Re_d = 30,000$ [198].

Figure 5.30: Computed streamlines for the Mach two case at a time of 1.75 μs.

One problem with level set methods is that they are not conservative. Dissipation introduced from advancing the level set equation changed the volume of the liquid in a non-conservative manner. The mass loss for the Mach two and Mach four cases are shown in Figure 5.31. At the end of the calculation, there is approximately 2.6% and 3.75% conservation error for the Mach two and Mach four cases respectively. This amount of conservation error is acceptable for the calculations in this work. Reducing the conservation error would
5.2.5 Interaction Between a Shock Wave and a Vaporizing Aluminum Droplet

In this section the interaction between a vaporization of an Al droplet and a shock wave is computed. Three shock-wave strengths are considered: none (quiescent), Mach two, and Mach four. The initial conditions for this case are shown in Figure 5.32; the shock waves propagate into air at a pressure of one atmosphere and a temperature of 300 K and the energy equation was solved in the liquid phase. To reduce the strength of the startup shock associated with impulsive vaporization, a layer of heated Al is initialized near the droplet using Eq. (3.125) with $Cr = 10^5$, $d = 1.25d_{Al}$, air at a temperature of 300 K, a pressure of one atmosphere, and zero velocity as the outside state that the shock wave propagates into, and an equilibrium Al vapor/air mixture at a temperature of 2750 K and zero velocity.

Figure 5.31: Computed (a) mass loss conservation error and (b) surface area for the heated droplet as a function of time.

require using six or more levels of refinement, which is impractical using the computational resources available to the author, especially when a reacting droplet is considered.

In terms of the progression of reflected and transmitted waves, droplet deformation, heat transfer, and separation angle the method interface coupling technique proposed in Chapter 4 is essentially verified and appears to work very well.
Figure 5.32: Initial conditions for the vaporizing and reacting Al droplet/shock wave interaction problem.

as the inside state. The top, left, and right boundary conditions are non-reflecting and the bottom boundary is an axis of rotation. The total height of the domain is $2.5r_{Al}$, which is high enough for the boundary conditions to not interfere with the vaporization of the droplet when a shock wave is considered, but does interfere with a quiescent case. These calculations are primarily to demonstrate applicability of the method and to compare and contrast the influence of shock wave on the vaporization of liquid droplets. Thus, the domain height is not increased for the quiescent case.

A time sequence for Mach two and Mach four shock waves are shown in Figures 5.33 and 5.34. The progression of the Schlieren field is quite similar to the non-vaporizing heated droplet for either shock-wave strength. The main difference is caused by larger heated layer near the droplet in the non-vaporizing case, which produces a different diffraction pattern. As the shock wave travels over the droplet, the pressure and high-speed flow simultaneously compress the Al vapor layer and strip it off the surface. The pressurization of the Al vapor near the surface does not change the equilibrium vapor pressure (since it is governed by the droplet surface temperature), but the equilibrium mass fraction is drastically reduced. Thus, the equilibrium vapor mass fraction is suddenly decreased and there is more Al vapor near the droplet surface than the new equilibrium condition allows and Al vapor locally condenses on the droplet surface. This produces a significant decrease in the total vaporization rate (shown in Figure 5.35) when the shock wave first impacts the droplet at about $t = 0.25 \mu s$ and $t = 0.125 \mu s$ for the Mach two and Mach four cases, respectively.

What is perhaps the most surprising result is that the rate of convection from the high speed gases behind the shock wave is not strong enough to make up for the reduction in vaporization rate from the shift in equilibrium vapor mass fraction. Recall from droplet
Figure 5.33: Time sequence of computed Schlieren and Al vapor mass fraction fields for a Mach two shock wave interacting with a 230 µm droplet at a temperature of 2750 K.

In vaporization theory, the average vaporization mass flux is:

\[ \dot{m}''_{\text{evap}} = \rho_g D \frac{\ln(1 + B)}{r}, \]  

(5.7)

where \( B \) is the Spalding transfer number, which is defined as:

\[ B = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}}. \]  

(5.8)

In the case of Al droplets, the molecular weight of air and Al vapor are very close, thus \( Y_v \approx X_v = p_v/p \). Then, assuming vapor partial pressure is zero far away from the droplet
and vapor pressure at the surface is saturated, the vaporization rate is:

$$\dot{m}_{\text{evap}}'' = \rho_g D \frac{\ln(p) - \ln(p - p_{\text{sat}})}{r}.$$  \hfill (5.9)
Shock waves not only increase pressure, but also introduce strong convective effects which enhance the rate of vaporization. One common method to estimate the increase of the vaporization rate from convection is to apply the Ranz-Marshall correlation \[40\]. Assuming a Lewis number of unity, the net rate of vaporization from a droplet is:

\[
\dot{m}_{\text{evap}}'' = \rho_g D \frac{\ln(p) - \ln(p - p_{\text{sat}})}{r} (1 + 0.267 \frac{R \Re_d^{1/2} P r^{1/3}}{D} ) .
\]

(5.10)

Then, the ratio of droplet vaporization from the quiescent to the shock-wave is:

\[
\frac{\dot{m}_\text{shock}''}{\dot{m}_\text{quiescent}''} = \frac{\ln(p_{\text{shock}}) - \ln(p_{\text{shock}} - p_{\text{sat}})}{\ln(p_{\text{quiescent}}) - \ln(p_{\text{quiescent}} - p_{\text{sat}})} (1 + 0.267 \Re_d^{1/2} P r^{1/3} ) .
\]

(5.11)

The shock wave does not influence the surface temperature (liquid shock waves are nearly isothermal), thus \(\rho_g D\) does not change when a droplet is impacted by a shock wave. Applying this expression for the Mach two case with a shock pressure of 7 MPa and a Reynolds number of 2,000 (evaluated at the surface temperature) gives the vaporization rate of the shock wave case to be 89% of the quiescent case (saturation pressure evaluated at 2750 K). Depending on how the Reynolds number and average pressure are selected, the ratio of the vaporization rate for the shock-wave case to the quiescent case can range between 0.75 and 1.05. After
the surface area increases from deformation, the total vaporization rate from the Mach four shock-wave case exceeds the quiescent case. It is interesting to note that the location corresponding to the strongest vaporization is not on the front stagnation point, but in the wake region where pressure is relatively low, as indicated by the mass fraction fields shown in Figures 5.36 and the pressure fields shown in Figure 5.37.

In the Mach four case, regions of low pressure form in the liquid droplet. This is primarily caused by the high rate of shear accelerating the liquid near the surface non-uniformly. Since the liquid is not assumed to be incompressible, the divergence-free condition does not hold. Thus, rarefaction waves can form in the droplet in regions with high shear, significantly reducing pressure or even inducing cavitation bubbles.
Table 5.3: Gaseous Al/O reaction mechanism used for shock wave/droplet interactions; $k_f = AT^n \exp(-E_a/R_aT)$.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>$A$ (mol/cm$^3$s)</th>
<th>$n$</th>
<th>$E_a$ (cal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Al + O$_2$ ⇌ AlO + O</td>
<td>$9.72 \times 10^{13}$</td>
<td>0.0</td>
<td>159.95</td>
</tr>
<tr>
<td>2</td>
<td>Al + O + M ⇌ AlO + M</td>
<td>$3.00 \times 10^{17}$</td>
<td>-1.0</td>
<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>AlO + O$_2$ ⇌ AlO$_2$ + O</td>
<td>$4.62 \times 10^{14}$</td>
<td>0.0</td>
<td>19885.90</td>
</tr>
<tr>
<td>4</td>
<td>Al$_2$O$_2$ ⇌ AlO + AlO</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>117900.00</td>
</tr>
<tr>
<td>5</td>
<td>Al$_2$O$_2$ ⇌ Al + AlO$_2$</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>148900.00</td>
</tr>
<tr>
<td>6</td>
<td>Al$_2$O$_2$ ⇌ Al$_2$O + O</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>104249.94</td>
</tr>
<tr>
<td>7</td>
<td>AlO$_2$ ⇌ AlO + O</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>88549.86</td>
</tr>
<tr>
<td>8</td>
<td>Al$_2$O ⇌ AlO + Al</td>
<td>$1.00 \times 10^{15}$</td>
<td>0.0</td>
<td>133199.94</td>
</tr>
<tr>
<td>9</td>
<td>O$_2$ + 4AlO → 2Al$_2$O$_3$(l)</td>
<td>$1.00 \times 10^{26}$</td>
<td>0.0</td>
<td>0.00</td>
</tr>
</tbody>
</table>

5.2.6 Interaction Between a Shock Wave and a Reacting Aluminum Droplet

The initial conditions for these problems were identical to the vaporizing droplet. The calculation consisted of nine species: Al, O$_2$, O, AlO, AlO$_2$, Al$_2$O, Al$_2$O$_2$, Al$_2$O$_3$(l), and N$_2$. To significantly reduce the number of species and chemical reactions, aluminum nitridation reactions and NOx formation are not considered. The chemical reaction mechanism presented in Table 2.1 was found to be numerically very stiff (i.e., there is a large discrepancy between the eigenvalues for the source term Jacobian) and gave both DVODE and CHEMEQ2 significant difficulty for the diffusion flame. Thus, the alumina condensation mechanism of Gallier et al. [39] was adopted to reduce stiffness of the source term vector. Note that there are significant typographical errors in their reaction mechanism and their entire reaction mechanism cannot be utilized. The reaction mechanism used for these calculations is given in Table 5.3. While the alumina condensation reaction is unusual, it has been shown to produce a proper flame temperature and diffusion flame structure [39] and does not posses the stiffness problems with the originally proposed reaction mechanism. The source term was integrated using CHEMEQ2 with four corrector stages and an error tolerance of $10^{-8}$.

As with the pure vaporization problem, the low height of the domain does affect the calculation at later times as shown in Figure 5.38. The velocity magnitude and other variables should be spherically symmetric, but are not due to the upper boundary condition. Again, the purpose of these calculations is mainly to demonstrate the applicability of the developed numerical techniques and to examine the effect of a shock wave on the diffusion flame structure and the vaporization rate.
The calculated diffusion flame structure for the quiescent case at the right side of the droplet along the centerline of the domain is shown in Figure 5.39 at a time of 1.05 $\mu$s. Due to the short amount of time that has elapsed, only a very small fraction of alumina has been formed and the AlO concentration peak is only around 0.4 droplet radii away from the surface, while Bucher et al. [200] measured the AlO peak to be around two droplet radii away from the surface. The reason for the large difference between the calculation and the empirical measurements are the short time scales in this thesis. Thus, a quasi-steady flame is not computed and a direct comparison to the data of Bucher et al. [200] is not appropriate. If the calculation was performed for a much longer time period and quasi-steady flame condition was met, the computed AlO peak would move further away from the droplet surface and computations could be compared directly to experimental data.

Contour plots of the temperature and species mass fractions of a Mach two shock wave interacting with a reacting Al droplet at a time of 2.13 $\mu$s is shown in Figure 5.40 and the pressure field is shown in Figure 5.41. The surface mass fraction of Al vapor is relatively unchanged from the non-reacting case. However, the concentration gradient of Al vapor at the surface is much greater due to very fast chemical reactions, which increases the rate of vaporization and produces a region of high temperature near the droplet. The shock wave increases the burning rate (shown in Figure 5.42) of the droplet which is opposite to the non-reacting case. It is expected that a normal fuel droplet such as (kerosene or methanol) would not behave in this manner, since chemical reactions involving those fuels tend to progress much more slowly and their boiling points are significantly lower. Many of the intermediate chemical species have their peak concentration in the boundary layer on the surface of the
droplet. Also note that there that a small amount of alumina is collecting in the boundary layer at the front stagnation point.

The result that a shock wave decreases the net vaporization rate for an inert droplet while increasing the net vaporization rate for a reacting aluminum droplet is not explainable from diffusion-limited droplet combustion theory. This suggests that the combustion of Al droplets in high-speed flows may be kinetic limited due to the high rate of convection, which in agreement with the recent experimental results of Tanguay et al. [34] where the combustion of Al particles was studied in high-velocity detonation products. In future extensions to this work, great care must be taken in selecting the homogeneous and heterogeneous chemical reaction mechanisms since they can greatly affect computed results in kinetically-controlled situations.

The computed pressure field for the reacting droplet (shown in Figure 5.41) is similar to the inert and purely vaporizing cases, with a peak pressure a little over eight atmospheres at the front stagnation point. While the increased pressure will locally increase the boiling point to around 3350 K, the increased boiling point does not change the fundamental vaporization

Figure 5.39: Calculated diffusion flame structure for a reacting Al droplet in a quiescent environment at a time of 1.05 $\mu$s.
Figure 5.40: Computed temperature and mass fraction fields for a Mach two shock wave interacting with an Al droplet at a time of 2.13 µs.
mechanism in this calculation. The droplet is not boiling before the arrival of the shock wave and saturation pressure is not changed by shock waves (saturation pressure is a function of liquid surface temperature, which is not influenced directly by shock waves). The shock wave could change the vaporization mechanism from being governed by the rate of energy entering the droplet (i.e., a boiling condition) to being governed by the equilibrium saturation vapor pressure if the droplet was assumed to be at the boiling condition at the start of the calculation. If the change in pressure is increased to a high value (around 100 atm in air), the boiling point may significantly exceed the flame temperature (as shown in Figure 1.7b) and the Al droplet will likely burn in a heterogeneous manner [201]. Pressures this high were not observed in this thesis, but could easily be obtained if the calculation considered Al droplets burning in the early stages of the post-detonation process of the HEX charge.

It is not practical to march the calculation until the droplet is completely vaporized since the time-step size is on the order of 87 ps. Using diffusion-limited droplet combustion and vaporization theory, the life time of the droplet can be estimated as:

$$t_b = \frac{\rho_l d_{Al}}{4 \dot{m}''}.$$  \hspace{2cm} (5.12)

The computed life time of the Al droplet using the mass flux at the end of the vaporization and reacting calculations is shown in Figure 5.43 along with the raw data compiled by Beckstead [14]. Most of the computed droplet life times are within the data scatter; however, the burning time of the reacting Al droplet impacted by a Mach two shock wave is a little lower. One possible reason for this is that none of the experiments measured the burning
time of Al droplets in an environment with shock waves. Also, the high relative velocity
between the droplet and the gas exists for a short time duration, thus using vaporization
rates while the convection rate is high would likely underestimate the burning time. It is
expected that the burning time of the reacting Al droplet in the quiescent environment
would increase as the diffusion flame moves away from the droplet surface. It is perhaps
tempting to determine the impact of convection on the mass burning rate of the droplet in
a form used by Gallier et al. [39] where \( \dot{m}_{Al,Re_d} = \dot{m}_{Al,Re_d=0}[1 + aRe_d^{b}Sc^c] \); however, with
the high speed flows considered in this thesis there is a significant increase in pressure from
the shock wave and variations in pressure around the surface of the droplet, which alter
both the total and local vaporization rates due to changes in the equilibrium mole fraction.
A simple Ranz-Marshall correction factor cannot account for the change a rate change of
droplet vaporization from a quiescent environment to a shock-wave induced flow. There
may be also be significant deformation of the droplet, which is definitely not accounted by
a simple Ranz-Marshall correction.

Considering the short time duration and complexity of the calculations presented in this
chapter, the developed numerical techniques perform very well for a variety of dynamic
compressible, multiphase, and/or reacting flows.
Figure 5.43: Comparison of the computed Al droplet life times to empirically measured burning times compiled by Beckstead [14].
CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

In this work a model of a shock wave interacting with a reacting Al droplet was developed. The model accounts for compressibility effects of both the gas and liquid phases. Phenomena included in this model that have not been accounted for in previous Al particle combustion models include: droplet deformation, liquid cavitation, wave propagation in the liquid phase, partial slip conditions at the surface, and the Marangoni stress. The level set method was used to separate the domain into gas-phase and liquid-phase regions and capture the deforming interface.

To compute the solution, a hybrid low-dissipation multi-component flux evaluation scheme was developed to calculate the chemically reacting gas-phase region with high and/or low Mach number features where $\gamma = \gamma(Y_i, T)$. The developed hybrid scheme combines characteristic and primitive variable interpolation using the low-dissipation nonlinear error controlled WENO method of Taylor et al. [202] in conjunction with the adaptive TVD slope limiting method of Kang et al. [138], the Low-Mach number adjustment of Thornber et al. [140], and the quasi-conservative double-flux multi-component of Billet and Abgrall [77] in conjunction with the AUSM$^{+}$-up flux [123]. The developed numerical scheme has the ability to perfectly preserve pressure and velocity when applied to material interfaces while
avoiding sharp temperature spikes and pressure oscillations produced by fully conservative methods. The scheme is relatively oscillation free exhibiting low-amplitude long-wavelength oscillations near shock waves, and has significantly reduced transverse shock anomalies by using a rotated Riemann solver adapted from Huang et al. [130]. When used to simulate the Richmyer-Meshkov instability, the fifth-order hybrid scheme produces flow-field structures that are comparable to similar calculations using ninth-order WENO [188]. It is demonstrated in this thesis that the gas-phase scheme can successfully calculate chemically reacting flows such as premixed deflagrations, Chapman-Jouget detonations, multi-dimensional detonations, and interactions between diffusion flames and shock waves. The technique presented in this thesis is relatively simple to implement from an existing compressible, Navier-Stokes solver based on Godunov’s method, and would be relatively straight-forward to extend to three-dimensional cases.

To couple the interface between a vaporizing and compressible liquid droplet to a compressible reacting gas, an extended Riemann problem was derived and solved exactly. This Riemann problem accounts for velocity jumps due to phase change and pressure jumps due to both surface tension and recoil pressure at the interface. The Riemann problem is solved exactly at the interface and used to populate ghost cells. The parabolic terms were coupled by directly calculating the diffusion fluxes and viscous stresses at the interface using jump conditions at an interface. In one dimension, computed results using this interface coupling technique compares very well with exact solutions. When applied to heated droplets, the computed results compared well with empirical measurements including: location boundary layer separation points, heat transfer correlations, and the qualitative shape of deformed droplets, indicating success of the method.

When the gas-phase and interface coupling techniques developed in this work were applied to a vaporizing droplet, the results indicate that shock waves decrease vaporization rate of droplets when compared to the quiescent case. The physical reason for this result is that the increased pressure from the shock wave decreases the vaporization rate more than convection induced by the high-speed flow behind the shock wave increases the vaporization rate, which is explainable using diffusion-limited droplet vaporization theory. Due to very fast chemical reactions between aluminum vapor and oxygen, shock waves were observed to increase the burning rate of the Al droplet considered, which not explainable from diffusion-limited droplet vaporization theory and suggests that Al droplets may burn in a kinetically-controlled manner when subjected to high-speed flows. The estimated droplet life times are
close to measurements of Al particle burning times, indicating that the numerical methods developed in this thesis perform well for complex situations.

The high-fidelity numerical methods developed in this work can be utilized in the future to explore fundamental physical phenomena involving multiphase compressible reacting flows. Applications to engineering systems can involve heterogeneous explosives, liquid-fueled pulse detonation engines, and among many others. To the author’s knowledge, this thesis is the first time that a compressible reacting gas-dynamic flow has been coupled to a compressible cavitating liquid with vaporization and surface tension effects.

6.2 Recommendations for Further Study

Although significant advancements in modeling techniques for reacting, and multiphase flows have been made in the work, there are many extensions that can be made in the future. When the interfacial coupling technique was applied to small droplets on fine grids, the number of Runge-Kutta-Chebyshev stages had to be increased by two in an ad-hoc manner to ensure stability. It would be useful to derive a stability criterion for the interfacial parabolic coupling technique to avoid this problem.

Another issue is the mass loss from the level set method. The mass loss did not effect the computations in this work too greatly, but may reduce the quality of the results if the Weber number of the droplet is higher. Much of the mass loss is likely caused the construction of the extension velocity at the surface using first-order extrapolation methods. It would be useful to use a higher-order extrapolation method in an attempt to reduce this error.

When the software library developed in this work was applied to the very stiff chemistry associated with Al diffusion flames, DVODE and CHEMEQ were found to be unreliable and the Al reaction mechanism proposed in Table 2.1 had to be changed to a less stiff reaction mechanism. A slightly less stiff chemical reaction mechanism was found to be much more stable for both DVODE and CHEMEQ. Since CHEMEQ was found to be unstable for particle drag calculations with small particles, to overcome this problem a different ODE integrator should be adopted.

To obtain more accurate results for vaporizing and reacting droplets in a quiescent environment, it would be useful to enlarge the domain and run the model for a longer time to establish a steady flame. Then, the estimated burning time of an Al droplet can be more fairly compared to experimental measurements in the quiescent case. Formal grid
convergence studies on shock wave and liquid droplet interactions were not performed due to resources available to the author, time constraints, and long queue times and fair share policies on PSU’s larger computing clusters. In the future, it would be useful to increase the refinement level of the mesh.
A.1 Thermodynamic Properties of Ideal Gas Mixtures

A.1.1 Multi-component Ideal Gas Law

In this work it is assumed that each gaseous component is in thermal equilibrium with all the other gaseous components and that each chemical species is treated as an ideal gas at its partial pressure, \( p_i \):

\[
p_i = \rho_i \frac{R_u}{M_{w_i}} T = [X_i] R_u T, \tag{A.1}
\]

where \( R_u \) is the universal gas constant, \( T \) is the temperature of the gas and \( M_{w_i} \), \( \rho_i \), and \( [X_i] \) are the molecular weight, density, and molar concentration of species \( i \), respectively. Dalton’s law of partial pressures states that:

\[
p = \sum_{i}^{N_g} p_i, \tag{A.2}
\]

where \( N_g \) is the number of gaseous chemical species.
This leads to the multi-component ideal gas law:

\[ p = \rho R_u T \sum_{i}^{N_g} \frac{Y_i}{Mw_i}. \]  
(A.3)

### A.1.2 Mass and Mole Fractions

The mass fraction of chemical species \( i \), \( Y_i \), is defined by:

\[ Y_i = \frac{\rho_i}{\rho} \]  
(A.4)

and by definition,

\[ \sum_{i=1}^{N_g} Y_i = 1 \]  
(A.5)

Similarly, the mole fraction of species \( i \), \( X_i \), is defined by the molar concentrations of the chemical species rather than their densities:

\[ X_i = \frac{[X_i]}{\sum_{k=1}^{N_g} [X_k]} \]  
(A.6)

The mass and mole fractions are related by:

\[ X_i = Y_i \frac{Mw_{mix}}{Mw_i} \]  
(A.7)

where the mixture molecular weight, \( Mw_{mix} \), is defined by

\[ Mw_{mix} \equiv \sum_{i=1}^{N_g} X_i Mw_i = \frac{1}{\sum_{i=1}^{N_g} Y_i / Mw_i} \]  
(A.8)

### A.1.3 Internal Energy, Specific Heat, and Entropy

In the gas phase, each chemical species is assumed to be thermally perfect, where the enthalpy and internal energy are functions of temperature only. The specific enthalpy, \( h_i \), and internal energy, \( e_i \), are defined as:

\[ h_i(T) = h_{f,i}^0 + \int_{T_0}^{T} C_p i(s) ds \]  
(A.9)
and
\[ e_i(T) = e_{f,i}^0 + \int_{T_0}^T C_{vi}(s) ds, \]  
(A.10)

where \( h_{f,i}^0 \) and \( e_{f,i}^0 \) are the standard enthalpy and energy of formation of species \( i \) at temperature \( T_0 = 0 \) K. The specific heats and standard entropies \( S_{i}^\circ \) for each species are evaluated using piecewise polynomial fits of the form
\[
C_{pi}(T) = \frac{R_u}{Mwi} \sum_{k=1}^{5} a_k T^{i-3},
\]  
(A.11)

\[
S_{i}^\circ = \frac{R_u}{Mwi} \left[ a_1 \ln(T) + \sum_{k=2}^{5} a_k T^{k-1} + a_7 \right],
\]  
(A.12)

where the polynomial coefficients are obtained from the compiled data of Goos et al. [203].

The mixture internal energy, enthalpy, and specific heats are given by:
\[
\xi = \sum_{k=1}^{N_g} Y_i \xi_i,
\]  
(A.13)

where \( \xi \) represents any mass weighted property.

Total specific internal energy, \( E \), is:
\[
E = \sum_{i}^{N_g} Y_i \left( h_{f,i}^0 + \int_{T_0}^T C_{pi}(s) ds \right) - \frac{p}{\rho} + \frac{\mathbf{v} \cdot \mathbf{v}}{2}.
\]  
(A.14)

### A.1.4 Speed of Sound

Another important property of the gas phase is the speed of sound defined by:
\[
c = \sqrt{\left. \frac{\partial p}{\partial \rho} \right|_{s,Y_1,\ldots,Y_{N_g}}},
\]  
(A.15)

which for an ideal gas is
\[
c = \sqrt{\gamma \frac{p}{\rho}},
\]  
(A.16)
where the specific heat of the mixture is defined as

$$\gamma = \frac{C_p}{C_v}.$$  \hspace{1cm} (A.17)

### A.1.5 Evaluation of Temperature

One aspect of compressible reacting flows is that temperature and pressure are not explicitly calculated in the governing equations; only the conserved variables are calculated. The primitive variables including pressure and temperature must be calculated since thermodynamic properties, transport properties, and chemical reaction rates need them. The temperature and pressure can be decoded from the conserved variables by using the equation of state and the definitions of internal energy and enthalpy, $h = e + p/\rho$. The pressure can be calculated from:

$$p = \rho h + \rho e = \rho \sum_i^{N_g} Y_i h_i(T) - \rho E + \frac{\rho U^2}{2}.$$  \hspace{1cm} (A.18)

Subtracting the ideal gas law, Eq. (A.3), from Eq. (A.18) gives an implicit relationship for temperature:

$$\phi(\rho, E, Y, T) = \rho \sum_i^{N_g} Y_i h_i(T) - \rho E + \frac{\rho U^2}{2} - \rho R_u T \sum_i^{N_g} \frac{Y_i}{M_{w_i}} = 0.$$  \hspace{1cm} (A.19)

Taking the temperature derivative of Eq. (A.19) while holding the density, velocity, composition, and internal energy constant gives:

$$\phi'(\rho, E, Y, T) = \frac{\rho R_u}{M_{w_{\text{mix}}} (\gamma - 1)}.$$  \hspace{1cm} (A.20)

Equation (A.19) is solved iteratively using the Newton-Raphson method with a convergence criterion of $10^{-9}$ unless otherwise noted

$$T^{i+1} = T^{i} - \frac{\phi(\rho, E, Y, T^i)}{\phi'(\rho, E, Y, T^i)}.$$  \hspace{1cm} (A.21)

Convergence typically requires less than ten iterations.
A.2 Gas Phase Chemical Kinetics

A chemical reaction mechanism with $N_R$ chemical reactions is:

$$\sum_{i=1}^{N_g} v_{ji}^f Z_k = \sum_{i=1}^{N_g} v_{ji}^r Z_k \quad (j = 1, \ldots, N_R),$$  \hspace{1cm} (A.22)

where $Z_k$ represents the name of species $k$. The parameters $v_{k,j}^f$ and $v_{k,j}^r$ represent the stoichiometric coefficients of species $k$ for the $j^{th}$ reaction in the forward and reverse directions respectively. The rate of progress for reaction $j$, $q_j$, is:

$$q_j = k_{f,j}^{\text{rate}} \prod_{k=1}^{N_g} [X_k]^{v_{k,j}^f} - k_{r,j}^{\text{rate}} \prod_{k=1}^{N_g} [X_k]^{v_{k,j}^r},$$  \hspace{1cm} (A.23)

where $k_{f,j}$ and $k_{r,j}$ are the forward and reverse reaction rate constants.

Some reactions require a third body for the reaction to proceed. One example of such a reaction is:

$$\text{Al} + \text{O} + \text{M} \rightleftharpoons \text{AlO} + \text{M},$$  \hspace{1cm} (A.24)

where the third body, $M$, is any collisional partner. In these reactions the concentration of the third body is calculated by:

$$\sum_{k=1}^{N_g} \alpha_{k,j} [X_k],$$  \hspace{1cm} (A.25)

where multiplier $\alpha_{k,j}$ represents the third body efficiency of species $k$ for reaction $j$. Unless otherwise noted, the value of a third body is assumed to be unity.

The forward rate coefficient is calculated using an Arrhenius form:

$$k_{f,j}^{\text{rate}} T = A T^{\beta} \exp(-E_a/R_u T),$$  \hspace{1cm} (A.26)

where $A$ is the pre-exponential factor, $\beta$ is the temperature exponent, and $E_a$ is the activation energy. The reverse rate is determined using the definition of the equilibrium constant,

$$K_{cj} \equiv \frac{k_{f,j}^{\text{rate}}}{k_{r,j}^{\text{rate}}},$$  \hspace{1cm} (A.27)
and the fact that equilibrium constant can be calculated from thermodynamic properties:

\[ K_{cj} = \exp \left( \frac{\Delta S_j^o}{R_u} - \frac{\Delta H_j^o}{R_u T} \right) \sum_{k=1}^{N_g} \left( \frac{p_o}{R_u T} \right) \sum_{i=1}^{N_g} \left( \nu_{r,j}^i - \nu_{f,j}^i \right), \]  
(A.28)

where \( p_o \) is the standard state pressure (1 bar) and

\[ \Delta H_j^o = \sum_{k=1}^{N_g} H_j^o(\nu_{r,j} - \nu_{f,j}^i), \]  
(A.29)
\[ \Delta S_j^o = \sum_{k=1}^{N_g} S_j^o(\nu_{r,j} - \nu_{f,j}^i). \]

Once the rates of progress are known for each chemical reaction, the rate of progress of species \( i \) is given by:

\[ \dot{\omega}_i = M_w \sum_{j=1}^{N_R} \left( \nu_{j,i}^r - \nu_{j,i}^f \right) q_j. \]  
(A.30)

### A.3 Gas Phase Transport Properties

In this section features of the kinetic theory of gases relevant to transport property evaluation will be summarized. More details are in Kee et al. [35] and Ern and Giovangigli [204]. In this work simplified routines will be used to evaluate the transport coefficients rather than using full multi-component relations based on Chapman-Enskog theory [35, 204] to save considerable computational expense.

#### A.3.1 Kinetic Theory Primer

The gaseous transport properties calculated in this work assume that the intermolecular potential function is given by the Stockmayer potential:

\[ u_{ij}(r_{ij}) = 4\epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} - \delta_{ij}^* \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{3} \right], \]  
(A.31)

where the collision diameter of nonpolar molecule \( i \) interacting with polar molecule \( j \) is:

\[ \sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \xi^{-1/6}, \]  
(A.32)
Table A.1: Coefficient for collision integral approximations.

<table>
<thead>
<tr>
<th>$j$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_j$</td>
<td>1.0458</td>
<td>0.15504</td>
<td>0.55909</td>
<td>2.1705</td>
<td>0.093193</td>
<td>1.5</td>
</tr>
<tr>
<td>$b_j$</td>
<td>1.0413</td>
<td>0.11930</td>
<td>0.43628</td>
<td>1.6041</td>
<td>0.095661</td>
<td>2.0</td>
</tr>
</tbody>
</table>

the well-depth parameter is:

$$
\epsilon_{ij} = \xi^2 \sqrt{\epsilon_i \epsilon_j},
$$

and the dipole-dipole interaction factor is:

$$
\tilde{\delta}_{ij} = \frac{1}{2} \frac{\mu_j \mu_i}{\epsilon_{ij} \sigma_{ij}^3},
$$

and

$$
\xi = 1 + \frac{1}{4} \frac{\alpha_i \mu_j}{\sigma_i^3 \sqrt{\epsilon_i \sigma_j^3}}.
$$

If molecules $i$ and $j$ are both polar or nonpolar, $\xi = 1$. The collision diameters, $\sigma_i$; well depth parameters, $\epsilon_i$; dipole moments, $\mu_i$; and polarizability, $\alpha_i$, of the molecules are model inputs.

The collision integrals used to evaluate the transport properties are approximated as:

$$
\Omega_{ij}^{(1,1)*} = \left[ 1 + \frac{(e^{a_5/T^*} - e^{-a_6/T^*})(\tilde{\delta}_{ij}^*)^2}{2 + 2.5 \tilde{\delta}_{ij}^*} \right] \left[ a_1 T^{*-a_2} + (T^* + a_3)^{-a_4} \right],
$$

$$
\Omega_{ij}^{(2,2)*} = \left[ 1 + \frac{(e^{b_5/T^*} - e^{-b_6/T^*})(\tilde{\delta}_{ij}^*)^2}{2 + 2.5 \tilde{\delta}_{ij}^*} \right] \left[ b_1 T^{*-b_2} + (T^* + b_3)^{-b_4} \right],
$$

where the reduced dipole moment was given above and the reduced temperature is given by:

$$
T^* = \frac{T k_B}{\epsilon}.
$$

The coefficients for the collision integrals are given in Table A.1.
Table A.2: Kinetic theory inputs for transport property evaluation. Note: 1 Debye = $3.1623 \times 10^{-25} \sqrt{m^5 kgs^{-1}}$.

<table>
<thead>
<tr>
<th>Name</th>
<th>L</th>
<th>$\epsilon/k_B$ (K)</th>
<th>$\sigma$ (Å)</th>
<th>$\mu$ (Debye)</th>
<th>$\alpha$ ($\text{Å}^3$)</th>
<th>$Z_{\text{rot}}$ (298)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>0</td>
<td>2750.000</td>
<td>2.6555</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>[205]</td>
</tr>
<tr>
<td>AlO</td>
<td>1</td>
<td>542.000</td>
<td>3.369</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>[205]</td>
</tr>
<tr>
<td>Al$_2$</td>
<td>1</td>
<td>2750.000</td>
<td>2.940</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>[205]</td>
</tr>
<tr>
<td>Al$_2$O$_2$</td>
<td>2</td>
<td>2750.000</td>
<td>3.5567</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>estimated</td>
</tr>
<tr>
<td>Al$_2$O</td>
<td>2</td>
<td>2750.000</td>
<td>3.3408</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>estimated</td>
</tr>
<tr>
<td>AlO$_2$</td>
<td>1</td>
<td>2750.000</td>
<td>3.5567</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>estimated</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>2</td>
<td>2750.000</td>
<td>3.5567</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>estimated</td>
</tr>
<tr>
<td>O</td>
<td>0</td>
<td>80.000</td>
<td>2.750</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>[206]</td>
</tr>
<tr>
<td>O$_2$</td>
<td>1</td>
<td>107.400</td>
<td>3.458</td>
<td>0.000</td>
<td>1.600</td>
<td>3.800</td>
<td>[206]</td>
</tr>
<tr>
<td>N$_2$</td>
<td>1</td>
<td>97.530</td>
<td>3.621</td>
<td>0.000</td>
<td>1.760</td>
<td>4.000</td>
<td>[206]</td>
</tr>
</tbody>
</table>

A.3.2 Kinetic Theory Input Parameters

All of the kinetic theory parameters used for estimating transport properties are listed in Table A.2. For some of the more exotic molecules, such as Al$_2$O, Stockmayer potential parameters have to be estimated using various rules listed in [35]. For a triatomic molecule the collision diameter can be estimated using

$$
\sigma_{ABC} = \frac{5}{12} \left[ \sigma_A + \sigma_B + \sigma_C \right] - 0.55.
$$

Unfortunately, the combining rules are not applicable to Al$_2$O$_2$ and Al$_2$O$_3$, so the kinetic theory parameters were simply taken to be those of AlO$_2$. The well depth parameter for all of the aluminum sub-oxides were taken to be that of Al since none of the estimation rules were applicable. Since the well depth parameter has less influence on transport properties than the collision diameter [205] and the sub-oxides are usually in small concentrations, the estimation of these parameters should not have much influence on the overall results of the model.
A.3.3 Shear Viscosity

The gas-phase mixture viscosity is given by [204]

\[ \mu = \left( \sum_{i=1}^{N_g} X_i \mu_i^{\frac{1}{6}} \right)^{\frac{6}{7}}, \]  

(A.39)

where the individual species viscosities are calculated using:

\[ \mu_i = \frac{5 \sqrt{\pi M_w i R u T}}{16 \pi \sigma_i^2 \Omega_{ii}^{(2,2)}}. \]  

(A.40)

A.3.4 Thermal Conductivity

The pure species thermal conductivities are given by [35]:

\[ \lambda_i = \frac{\mu_i}{M_w i} (f_{\text{trans}} C_{\text{vtrans}} + f_{\text{rot}} C_{\text{vrot}} + f_{\text{vib}} C_{\text{vib}}), \]  

(A.41)

where

\[ f_{\text{trans}} = \frac{5}{2} \left(1 - \frac{2}{\pi} \frac{C_{\text{vrot}}}{C_{\text{vtrans}}} \frac{A}{B}\right), \]  

(A.42)

\[ f_{\text{rot}} = \frac{\rho D_{ii}}{\mu_i} \left(1 + \frac{2}{\pi} \frac{A}{B}\right), \]  

(A.43)

\[ f_{\text{vib}} = \frac{\rho D_{ii}}{\mu_i}, \]  

(A.44)

\[ A = \frac{5}{2} - \frac{\rho D_{ii}}{\mu_i}, \]  

(A.45)

\[ B = Z_{\text{rot}} + \frac{2}{\pi} \left(\frac{5}{3} \frac{C_{\text{vrot}}}{R_i} + \frac{\rho D_{ii}}{\mu_i}\right). \]  

(A.46)

The translational specific heat of a gas is given by:

\[ C_{\text{vtrans}} = \frac{5}{2} R_u, \]  

(A.47)
and the rotational specific heat is:

\[
C_{v_{\text{rot}}} = \begin{cases} 
0 & \text{(monatomic molecule, } L = 0) \\
R_u & \text{(linear molecule, } L = 1) \\
\frac{3}{2} R_u & \text{(nonlinear molecule, } L = 2). 
\end{cases}
\]  

(A.48)

The vibrational specific heat is calculated by subtracting the rotational and translational contributions from the total specific heat,

\[
C_{v_{\text{vib}}} = C_v - C_{v_{\text{rot}}} - C_{v_{\text{trans}}}. 
\]  

(A.49)

In the case of monatomic molecules the vibrational specific heat is zero.

The rotational relaxation collision number, \( Z_{\text{rot}} \), is:

\[
Z_{\text{rot}}(T) = Z_{\text{rot}}(298) \frac{F(298)}{F(T)}, 
\]  

(A.50)

where the Parker correction factor, \( F \), is defined by:

\[
F(T^*) = 1 + \frac{\pi^{3/2}}{2} T^{*1/2} + \left( \frac{\pi^2}{4} + 2 \right) T^* + \pi^{3/2} T^{*3/2}. 
\]  

(A.51)

The self diffusion coefficient is:

\[
D_{ii} = \frac{3}{8} \frac{\sqrt{\pi R_u^3 T^3 / Mw_i}}{N_{Av} p \pi \sigma_k^2 Q_{ii}^{(1,1)*}}, 
\]  

(A.52)

where \( N_{Av} \) is Avogadro’s number.

The gas phase mixture thermal conductivity is calculated using the simplified method of Ern and Giovangigli [204]:

\[
\lambda = \left( \sum_{i=1}^{N_g} X_i \lambda_i^{1/4} \right)^4. 
\]  

(A.53)

### A.3.5 Volume Viscosity

In many simulations it is often assumed that Stoke’s hypothesis \( (\kappa = \beta - 2/3 \mu = 0) \) is valid. This assumption only true for dilute monatomic gases [207] and is usually invalid for
diatomic or polyatomic gases since the ratio of the volume to the shear viscosity is usually $O(1)$ [79], not 0 as Stokes hypothesis suggests. The inclusion of this property can have a significant impact on the shock induced vortex generation and smooths the flow field in situations with complicated shock interactions [79]. At any rate, researchers working with the compressible Navier-Stokes equations are always looking for reasons to add dissipation for stability reasons.

Although this fluid property is difficult to measure, kinetic theory can be used to calculate it for mixtures of ideal gases [204]. The individual species volume viscosity is approximated as:

$$\kappa_i = \frac{R_u\pi}{4} \left( \frac{Cv_i - Cv_{\text{trans},i}}{Cv_i} \right)^2 \max \left[ Z_{\text{rot}}(298), 1 \right] F(t) \frac{1}{F(298) Cv_{\text{rot},i}} \mu_i,$$

and the mixture-average volume viscosity is:

$$\kappa = \left( \sum_{i=1}^{N_g} X_i \kappa_i^{3/4} \right)^{\frac{4}{3}}.$$

The ratios of volume to shear viscosity for several gaseous species as a function of temperature are shown in Figure A.1. It is clear that Stoke’s hypothesis is incorrect for most of the gaseous species. Measurements of the viscosity ratio room temperature for N$_2$, H$_2$, CO, and CH$_4$ were at values of 0.73, 33.4, 0.55, and 1.33, respectively [79]; while the calculated values are 0.504, 33.8, 0.22, and 2.01. Although the calculated values are not perfect, they are fine considering the assumptions involved in their evaluation and are certainly better than assuming that they are all zero.

A.3.6 Binary Diffusion Coefficients

The binary diffusion coefficient is calculated using:

$$D_{ij} = \frac{3}{16} \sqrt{2\pi R_u^4 T^3 (Mw_i + Mw_j)/Mw_i Mw_j} \frac{N_A \rho \pi \sigma_{ij}^2 \Omega_{ij}^{(1,1)}}{\sigma_{ij}^*}.$$

In this work the Curtis-Hirschfelder approximation [35] is used to evaluate the mixture-average diffusion coefficient:

$$D_{i,\text{mix}} = \frac{1 - Y_i}{\sum_{j \neq i} N_g X_j / D_{ij}} \approx \frac{\sum_{j \neq i} N_g (X_j + \epsilon) Mw_j}{Mw_{\text{mix}} \sum_{j \neq i} (X_j + \epsilon) / D_{ij}},$$
where $\epsilon$ is a small parameter to avoid division by zero in the case where there is only one species present. More exact methods exist [35, 204], but they are computationally expensive, requiring the inversion of an $N^3 \times N^3$ matrix that is a function of local species composition, pressure, and temperature. Given the uncertainties involved when selecting kinetic theory input parameters, multi-component diffusion may not be much superior to less exact mixture averaged formulations.

A.3.7 Thermal Diffusion Coefficients

In situations where the Soret and Dufour effects are important, the thermal diffusion coefficients are needed. Should thermal diffusion ever be needed, the Ramshaw approximation [208] could be used. For mixtures of ideal gases, the Ramshaw approximation is:

$$
\frac{Mw_{\text{mix}}}{\rho Mw_i} \sum_{j \neq i} \frac{1}{Mw_j \bar{D}_{ij}} (Y_j \bar{D}_i^T - Y_i \bar{D}_j^T) = \sum_{j \neq i} (\alpha_{ji} - \alpha_{ij}),
$$

(A.58)
\[ \alpha_{ij} = F_{ij} \left( \sum_{i=1}^{N_g} \frac{Y_k}{Mw_k} \sigma_{jk}^2 \left( \frac{Mw_j + Mw_k}{Mw_j Mw_k} \right) \right)^{-1}, \]

\[ F_{ij} = \frac{1}{3} Y_i Y_j \sqrt{\frac{Mw_j Mw_k}{(Mw_j + Mw_k)^3}} \left( 10 \Omega_{ii}^{(1,1)*} - 12 \Omega_{ii}^{(1,2)*} \right). \]  

(A.59)

The collision integral \( \Omega_{ii}^{(1,2)*} \) can be calculated by [209]:

\[ \Omega_{ii}^{(1,2)*} = \frac{A}{T^*B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}, \]  

(A.60)

where \( A = 1.00220, B = 0.15530, C = 0.16105, D = 0.72751, E = 0.86125, F = 2.060848, G = 1.95162, H = 4.84492. \) While far simpler than Chapman-Enskog theory, the Ramshaw approximation is still expensive to evaluate since it requires the solution of a \( N_g \times N_g \) system of equations with a dense, unsymmetric matrix. Typically thermal diffusion is only important for light species such as H, H\(_2\), He, etc. For example, Pope and Gogos [210] found only a 2\% difference in the extinction velocity for methanol droplet when thermal diffusion was added. Due the expense and high molecular weight of the species involved with aluminum combustion, thermal diffusion is ignored in this work.

**A.4 Liquid Equation of State**

Since this model examines wave propagation processes in the liquid region, a compressible liquid equation of state must be used. Unfortunately, measurements on the critical properties of liquid aluminum are not reliable with cited values of critical temperature ranging from 5115 to 9333 \( K \) [211–213] and the critical properties of liquid alumina could not be found at all (likely because it dissociates before it vaporizes). Thus, more complete and complex real gas/liquid equations of state such as Peng-Robinson or Benedict-Webb-Rubin cannot be used in this work. Due to its simplicity, the equation of state used for liquid region is a variant of the Tait equation [82]:

\[ p = B \left( \frac{\rho}{\rho_0(T)} \right)^N - B + A, \]  

(A.61)
where \( A \) and \( \rho_0 \) are the reference pressure and density, respectively and \( B \) and \( N \) are constants. The unmodified Tait assumes that the reference pressure and density are constants, which removes any temperature dependence on the equation of state.

The speed of sound for any fluid, which can be derived from the acoustic wave equation and Maxwell’s relations, is:

\[
c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T + \frac{T \left( \frac{\partial p}{\partial T} \right) \rho}{C_v \rho^2}}. \tag{A.62}
\]

The specific heat \( C_p \) used in this work is 1177 J/kgK \cite{13}. The sound speed requires the constant volume specific heat, not the constant pressure. \( C_p \) and \( C_v \) are related by:

\[
C_p - C_v = \frac{T \alpha_T^2}{\rho \kappa_T}, \tag{A.63}
\]

where \( \kappa_T \) is the isothermal compressibility:

\[
\kappa_T \equiv \frac{1}{\rho} \frac{\partial \rho}{\partial p} \bigg|_T = \frac{1}{\rho} \frac{\partial p}{\partial \rho} \bigg|_T, \tag{A.64}
\]

and \( \alpha_T \) is the coefficient of thermal expansion:

\[
\alpha_T \equiv -\frac{1}{\rho} \frac{\partial \rho}{\partial T} \bigg|_p = \frac{1}{\rho} \frac{\partial p}{\partial T} \bigg|_p. \tag{A.65}
\]

Substituting the specific heat difference into Eq. (A.62) and realizing that

\[
\frac{\partial p}{\partial T} \bigg|_p = \frac{\partial p}{\partial \rho} \bigg|_T \frac{\partial \rho}{\partial T} \bigg|_p, \tag{A.66}
\]

gives:

\[
c = \sqrt{p_0 + \frac{T \left( \frac{\partial p}{\partial T} \right) \rho \left( \frac{\partial \rho}{\partial p} \right)_T^2}{\rho^2 C_p - T \left( \frac{\partial p}{\partial T} \right)_p^2 \left( \frac{\partial \rho}{\partial p} \right)_T}}. \tag{A.67}
\]

Applying this definition to the modified Tait equation produces:

\[
c^2 = \frac{N(p + B - A)}{\rho} + \frac{T}{C_v} \left[ \frac{NB}{\rho} \left( \frac{\rho}{\rho_0} \right)^N \frac{1}{\rho_0(T) dT} \right]^2. \tag{A.68}
\]
To complete the modified Tait EOS, a complementary calorific equation of state is needed to relate internal energy to temperature. By definition:

$$de = C_v dT + \left[ T \left( \frac{\partial p}{\partial T} \right)_v - p \right] dv.$$  \hspace{1cm} (A.69)

Using the modified Tait equation assuming constant specific heat, gives:

$$e = \left[ C_v + \frac{N}{N-1} \frac{p + B - A}{\rho} \frac{1}{\rho_0(T)} \frac{dp_0}{dT} \right] T + \frac{p + N(B - A)}{\rho(N-1)} + e_0.$$  \hspace{1cm} (A.70)

The formal expressions for the speed of sound and internal energy for the modified Tait equation are complex and are not compatible for the Riemann solver at the liquid gas interface. If the term involving $dp_0/dT$ is ignored, the expressions for sound speed and internal energy become more amenable to interfacial Riemann solvers:

$$c^2 = \frac{N(p + B - A)}{\rho},$$  \hspace{1cm} (A.71)

$$e = C_v T + \frac{p + N(B - A)}{\rho(N-1)} + e_0,$$  \hspace{1cm} (A.72)

$$h = e + \frac{p}{\rho} = C_v T + \frac{N(p + B - A)}{\rho(N-1)} + e_0.$$  \hspace{1cm} (A.73)

Schmidt et al. [83] used a similar simplification and found that although these simplified thermodynamic expressions do not satisfy Maxwell’s thermodynamic relations, the error introduced is small and does not seem to affect the overall calculated results.

For liquid mixtures there are not any obvious ways to develop a mixture Tait equation. In lieu of mixing rules for the Tait equation, Dymond and Malhotra [214] mix the $B$ parameter by the mole fractions of the species in the liquid mixture. Following this approach, all parameters and constants for the mixture Tait equation could be summed and weighted by the mole fraction:

$$N_{\text{mix}} = \sum X_i N_i,$$  \hspace{1cm} (A.74)
and similarly for the mixture $B$, reference pressure, and reference density. The mixture energy could be handled in the obvious manner:

$$e_{\text{mix}} = \sum_{i} Y_i e_i.$$  \hfill (A.75)

### A.5 Liquid Aluminum Thermodynamic and Transport Properties

There are several sources for liquid aluminum density, but only one covers the temperature range needed for this study, [215]. At $p_{\text{ref}} = 0.3$ GPa

$$\rho_{0.3 \text{ GPa}}(\text{kg/m}^3) = 2606 - 0.210T(K); \quad 933 \text{ K} < T < 4000 \text{ K} \quad \text{(A.76)}$$

The data used in the generation of the above correlation has $\pm 5\%$ uncertainty, meaning that at the melting temperature ($933K$) the density could lie anywhere between 2290 and 2530 kg/m$^3$. At atmospheric pressure, density measurements have been compiled by the Design Institute for Physical Property Data (DIPPR) [213] and Assael et al. [216]. These low pressure density correlations are:

$$\rho_{\text{atm}}(\text{kg/m}^3) = 2592.38 - 0.238T(K); \quad 933 \text{ K} < T < 1274 \text{ K} \quad \text{[213], (A.77)}$$

$$\rho_{\text{atm}}(\text{kg/m}^3) = 2667.39 - 0.311T(K); \quad 933 \text{ K} < T < 1190 \text{ K} \quad \text{[216], (A.78)}$$

Another property that is crucial to the success of this model is the sound speed of liquid aluminum. Blairs and Abbasi, [217] compiled ultrasound data and found that:

$$c(\text{m/s}) = 5132 - 0.466T(K); \quad 933 \text{ K} < T < 1273 \text{ K}. \quad \text{(A.79)}$$

Using the measured sound speed and the three density density correlations to estimate $\partial p/\partial \rho$ gave values from $1.698 \times 10^7$ to $1.941 \times 10^7$ m$^2$/s$^2$. However, using the density data directly, gives $\partial p/\partial \rho = 7.49 \times 10^6$ m$^2$/s$^2$ and a sound speed of 2790 m/s, which is far too low.

Since there are multiple sources that give the atmospheric liquid Al density at melting near the suggested value of DIPPR, the high pressure data was “corrected” to ensure that it is consistent with both the speed of sound measurements and the atmospheric density
Table A.3: Parameters used for the liquid aluminum and alumina Tait equation of state.

<table>
<thead>
<tr>
<th>Liquid</th>
<th>$A$(Pa)</th>
<th>$B$(Pa)</th>
<th>$N$</th>
<th>$C_p$(J/kgK)</th>
<th>$h_f^0$(J/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>101325</td>
<td>Eq. (A.81)</td>
<td>8.55</td>
<td>1177</td>
<td>$-2.9263 \times 10^5$</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>101325</td>
<td>$1.55 \times 10^{10}$</td>
<td>8.50</td>
<td>1883</td>
<td>$-1.7239 \times 10^7$</td>
</tr>
</tbody>
</table>

measurements. Changing the high pressure density correlation Eq. (A.76) to

$$\rho_{0.3 \text{ GPa}}(\text{kg/m}^3) = 2581.06 - 0.210T(K); \ 933 \text{ K} < T < 4000 \text{ K} \quad (A.80)$$

solves this inconsistency, while matching the accepted density at atmospheric pressure. This modification shifts the density by 1.1% at 933 K and 1.4% at 4000 K, which is well within the 5% uncertainty. Thus, the reference pressure for the modified Tait EOS is given by Eq. (A.80) at $p_{\text{ref}} = 0.3$ GPa.

Based on optimizing the values of $N$ and $B$ to match the sound speed and density correlations, $N$ was selected to be 8.55 and $B$ is given by:

$$B = 7.98876 \times 10^9 - 2.18423 \times 10^6T + 199.063T^2 - 0.00604723T^3 \quad (A.81)$$

where $T$ is the initial temperature of the liquid phase in Kelvin.

Now that the reference pressure and density have been selected; the parameters $N$, $B$, and $A$ can be selected by matching the speed of sound calculated by the Tait equation. A summary of the Tait parameters used in this work are given in Table A.3

The computed density and sound speed as a function of temperature for liquid Al at a pressure of $p = 0.3$ GPa are shown in Figure A.2.

The liquid aluminum saturation pressure needed for aluminum evaporation used in this work is given by [213]:

$$p_{\text{sat}}(\text{Pa}) = \exp \left[36.547 - \frac{39033}{T} - 1.3981 \ln(T) + 6.7839 \times 10^{-9}T^2 \right], \quad (A.82)$$

where $T$ is the surface temperature of the liquid in Kelvin.
Figure A.2: Comparison of computed (a) density and (b) sound speed as a function of temperature at $p = 0.3$ GPa using the Tait equation of state to the correlations. The dashed lines correspond to the uncertainty from Eq. (A.80).

Liquid Al Transport Properties

The thermal conductivity of liquid Al was determined as a function of temperature by Recoules and Crocombette [218],

$$\lambda(\text{W/mK}) = 42 + 0.056T(K); \quad 933 \text{ K} \leq T \leq 3000 \text{ K}. \quad (A.83)$$

Assael et al. [216] compiled data of Al shear viscosity measurements. Their suggested correlation is:

$$\mu(\text{Pas}) = 1.85183 \times 10^{-4} \exp\left(\frac{1850.1}{T(K)}\right); \quad 933 \text{ K} \leq T \leq 1270 \text{ K}. \quad (A.84)$$

Measurements or calculations on the volume viscosity of liquid aluminum could not be found. As discussed earlier, it is usually better to assume that this parameter is unity rather than zero. Thus, the volume viscosity ratio for liquid Al is assumed to be unity.

Surface tension measurements of liquid Al made and compiled by Sarou-Kanian et al. [219] at temperatures ranging 933 to $2170K$. They found the following correlation works well:

$$\sigma_t(\text{N/m}) = 1.27964 - 0.000274T(K); \quad 933 \text{ K} \leq T \leq 2170 \text{ K}. \quad (A.85)$$
Surface tension measurements also indicated a gaseous environment that the Al\(_{(l)}\) was placed in (e.g., He, Ar, or Ar/H\(_2\)) had a small influence. Thus, it is likely that Eq. (A.85) can safely be used for the gas mixtures considered in this work.

In the event that the temperature exceeds the bounds of any transport coefficient correlation, the transport properties will simply be extrapolated using the above correlations. Since all of the above correlations behave nicely outside of their range of validity and give reasonable values, this practice should not produce unphysical values.

### A.6 Liquid Alumina Thermodynamic and Transport Properties

Since alumina is a high-temperature refractory material, empirical measurements of its liquid thermodynamic and transport properties are extremely difficult. Often alumina is used as a crucible material to obtain high-temperature molten properties for other materials. Recently, electrostatic [220–222] and aerodynamic levitation methods [223, 224] have been used to obtain detailed thermodynamic and some transport properties of liquid alumina. The alumina density used in this work is [223]:

\[
\rho_{\text{Al}_2\text{O}_3(l)}(\text{kg/m}^3) = 3084.35 - 0.117738T(K); \quad 2000 \text{ K} \leq T \leq 3100 \text{ K}.
\] (A.86)

Measurements show that the specific heat of molten alumina is essentially constant, varying only 9 J/kgK from 2120 to 2450 K [220]. Thus, the specific heat will be taken to be the average value in this range \((C_p = 1883 \text{ J/kgK})\).

The speed of sound in liquid alumina has been measured by Sinn et al. [225] using inelastic X-ray scattering on aerodynamically levitated 3 to 4 mm alumina droplets. Their results indicated that the speed of sound in molten alumina is \(c = 7350 \text{ m/s}\) at 2323 K and \(c = 6530 \text{ m/s}\) at 3073 K. Since the alumina in the liquid phase region of the calculation is at a temperature close to the boiling point of aluminum, the alumina speed of sound used in this work is \(c_{\text{Al}_2\text{O}_3(l)} = 6530 \text{ m/s}\). A summary of the liquid alumina EOS parameters is given in Table A.3.

### Liquid Alumina Transport Properties

Glorieux et al. [224] measured the surface tension of liquid alumina by relating the frequency of oscillation of a perturbed aerodynamically levitated droplet and suggested the
following correlation:

\[ \sigma_t(N/m) = 0.7475 - 0.000039T(K); \quad 2327 \text{ K} \leq T \leq 3200 \text{ K.} \]  

(A.87)

Using a similar technique, Paradis et al. [221] measured the shear viscosity of molten alumina using the decay rate of an oscillating droplet:

\[ \mu(\text{Pas}) = 0.0032 \exp\left(\frac{5195.74}{T(K)}\right); \quad 2190 \text{ K} \leq T \leq 2500 \text{ K.} \]  

(A.88)

Using ab initio DFT molecular dynamics calculations, Jahn and Madden [226] found that the ratio of the volume to shear viscosity of molten alumina at 2350 K is 1.167.

Unfortunately, measurements or calculations of liquid alumina thermal conductivity could not be found at this time. In lieu of experimental measurements, Sinn et al. [225] assumed that the thermal conductivity of molten alumina was same value as high-temperature solid alumina (\(\lambda = 7.4 \text{ W/mK}\)). While this assumption is obviously not correct, Sinn et al. [225] point out that the transport processes (speed of sound, self diffusion, etc.) in liquid alumina are comparable to solid alumina. Thus, it would be reasonable to expect similar behavior for thermal conductivity.
B.1 Background

A generic conservation law can be written as:

$$\frac{\partial v}{\partial t} + \frac{\partial f}{\partial x} = 0,$$  \hspace{1cm} (B.1)

which can be solved numerically by using the method of lines with conservative spatial discretization of the flux gradient:

$$\frac{dv_i}{dt} + \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x} = 0.$$  \hspace{1cm} (B.2)

If the solution data is known at discrete points (finite difference) or is assumed to be cell averaged (finite volume), the fluxes at the cell edges are not inherent to the data and must be interpolated using various schemes that are both accurate and oscillation-free when discontinuities are present. This work utilizes the MUSCL and WENO class of schemes.

Achieving high-order spatial accuracy for hyperbolic conservation laws continues to be a very challenging problem since they allow discontinuous solutions. As mentioned in Chapter 3, the solution of hyperbolic conservation laws requires that the primitive variables, conserved variables, or split numerical fluxes to be interpolated to the cell edges in both the upwind and
downwind directions. Using traditional high-order interpolation schemes, such as Lagrangian interpolation [227, 228], will lead to spurious oscillations that destroy the quality of the solution when a discontinuity is present. On the other hand, if a first-order method is used spurious oscillations will not appear but any sharp features in the solution will be smeared by numerical dissipation.

Modern high-order numerical methods such as Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) [113, 114, 137, 229] or Weighted Essentially Non-Oscillatory (WENO) [119, 230] schemes use high-order interpolation when the solution is smooth for high accuracy and switch to low-order interpolation when sharp gradients are present to suppress oscillations.

B.2 MUSCL Schemes

One of the most popular edge interpolation schemes for hyperbolic conservation laws is the MUSCL scheme introduced by van Leer [229]. In its most general form, MUSCL schemes interpolate a variable, $u$, to cell edge $i + 1/2$ from the left via:

$$v_{L,i+1/2} = v_i + 0.5(v_i - v_{i-1})\phi(r_i, \alpha, \beta), \quad (B.3)$$

where $\phi$ is a slope limiter, $v_{L,i+1/2}$ is the left interpolated variable at cell edge $i + 1/2$, and the slope ratio $r_i$ is:

$$r_i = \frac{v_{i+1} - v_i}{v_i - v_{i-1}}. \quad (B.4)$$

The slope limiter changes the order of the interpolation from up to fifth to first depending if the function senses any short wavelength oscillations or discontinuities. There are many different forms for the slope limiters [137] including:

- minmod:

$$\phi(r_i, \alpha, \beta) = \max(0, \min(r_i, 1)), \quad (B.5)$$

- van Leer:

$$\phi(r_i, \alpha, \beta) = \max \left[ 0, \min \left( \alpha, \alpha r_i, \frac{2r_i}{1 + r_i} \right) \right], \quad (B.6)$$

- superbee:

$$\phi(r_i, \alpha, \beta) = \max[0, \min(\alpha r_i, 1), \min(r_i, \alpha)], \quad (B.7)$$
Third Order Multi-dimensional Limiting Process (MUSCL3):

\[
\phi(r_i, \alpha, \beta) = \max \left[ 0, \min \left( \alpha, \alpha r_i, \frac{1 + 2r_i}{3} \right) \right],
\]

(B.8)

Fifth Order Multi-dimensional Limiting Process (MUSCL5):

\[
\phi(r_i, \alpha, \beta) = \max \left[ 0, \min \left( \alpha, \alpha r_i, \frac{-2/r_{i-1} + 11 + 24r_i - 3r_ir_{i+1}}{30} \right) \right],
\]

(B.9)

among many others. In one dimension, the factor \(\alpha\) is approximately 2, in two dimensions it is defined to be [137]:

\[
\alpha = \max \left[ 1, \min \left( 2, \frac{2 \max(1, r_j)\left(1 + \max(0, r_{i+1}\tan \theta_{i+1})\right)}{1 + \tan \theta_i} \right) \right],
\]

(B.10)

where

\[
\tan \theta_i = \left| \frac{v_{i,j+1} - v_{i,j-1}}{v_{i+1,j} - v_{i-1,j}} \right|.
\]

(B.11)

If the interpolation is to a face in the \(y\)-direction, all of the above formulas can be applied by simply replacing grid index in the \(x\)-direction, \(i\), with the grid index in the \(y\)-direction, \(j\) and vice versa.

In general the Multidimensional Limiting Process (MLP) can be applied to any interpolation method including WENO by taking:

\[
\phi(r_i, \alpha, \beta) = \max \left[ 0, \min \left( \alpha, \alpha r_i, 2\frac{v_{L,i+1/2} - v_i}{v_i - v_{i-1}} \right) \right],
\]

(B.12)

where \(v_{L,i+1/2}\) is the original, unmodified interpolated variable. A comparison on effect of the slope limiter for MUSCL schemes on the scalar wave equation is shown in Figure B.4.

### B.3 WENO Schemes

WENO schemes have become very popular and currently enjoy great success in constructing advection schemes for hyperbolic conservation laws. Specific applications include the Euler equations of gas dynamics [119], solving the Hamilton-Jacobi and Eikonal equations associated with the level-set approach [54, 55], incompressible fluid flow [231], implicit large
eddy simulations of compressible turbulence [86] and a myriad of other applications with hyperbolic conservation laws.

The popularity of WENO stems from their high order of accuracy, schemes up to 17th-order accurate have been developed [119, 232]. While ninth-order accurate may seem excessive, it turns out these high-order schemes are usually more computationally efficient than lower-order (2nd or 3rd) methods. When fifth-order WENO (WENO5) was pitted against ninth-order WENO (WENO9) to simulate the standard two dimensional double Mach reflection and Rayleigh-Taylor instabilities, Shi et al. [233] found that grid spacing can be increased by about a factor of two with WENO9 and achieve a similar error to WENO5. Although WENO9 is around 30% more expensive in terms of CPU time per time step at a given node, the fact that coarser grids (and time step sizes) can be used translates a 66-80% reduction in computation time over WENO5. Latini et al. [188] and Thornber et al. [86] came to similar conclusions when comparing the effect of WENO order on simulation results of the Richtmyer-Meshkov instability and implicit large eddy simulations of homogeneous decaying turbulence, respectively.

B.3.1 Derivation of WENO schemes

The following derivation closely follows that of Cockburn et al. [230]. Consider cell averaged data shown in Figure B.1. To construct a conservative scheme, the data, $v(x)$, cannot be interpolated directly but must be cast into conservative (or primitive) form, which is denoted as $V(x)$. This is done by appealing to the original conservation law and integrating the data over space:

$$V(x) = \int_{-\infty}^{x} v(\xi) \, d\xi.$$  (B.13)
Using the fact that the data are cell averaged:

\[ V(x_{i+1/2}) = \int_{-\infty}^{x} v(\xi) \, d\xi \]
\[ = \sum_{j=-\infty}^{i} \int_{x_{j-1/2}}^{x_{j+1/2}} v(\xi) \, d\xi \]
\[ = \sum_{j=-\infty}^{i} v_j \Delta x_j. \]  

(B.14)

Thus, the primitive is known exactly at the cell centers. A conservative interpolation scheme is formed by fitting a Lagrangian interpolation polynomial through the primitive at these locations. The interpolation polynomial of the original data is found by taking the derivative of the primitive interpolation function. Ultimately, we want to find

\[ v(x_{i+1/2}) = \sum_{j=0}^{r-1} a_j^r v(x_{i-u+j}), \]  

(B.15)

where \( r \) is the number of original data points used in the interpolation.

Before constructing the polynomial, we need to consider the stencil: data in \( u \) cells in the upwind direction and \( d \) cells in the downstream direction in addition to the cell that contains the edge in the upwind direction are used to interpolate the data at \( x_{i+1/2} \). Basic numerical analysis states that there is a unique polynomial of degree \( r = u + d + 1 \) that will give the same cell average as the original data. Referring to Figure B.1, blue are cells used in the polynomial construction. Since the interpolation is from the left, the upwind cell \( i \) contains cell-edge \( i + 1/2 \), thus and \( u = 2 \) and \( d = 1 \) in this particular case. Had the interpolation been from the right and the same cells used for the interpolation, the upwind cell containing the edge would be cell \( i + 1 \), \( u \) would be zero, and \( d \) would be three.

The polynomial of the primitive is constructed by forming a Lagrangian interpolation polynomial, \( P(x) \), through the cell edge values. The details of Lagrangian interpolation can be found in any standard text on numerical analysis [227, 228, 234]:

\[ P(x) = \sum_{m=0}^{r} V(x_{i-u+m-1/2}) \prod_{l=0}^{r} \frac{x - x_{i-u+l-1/2}}{x_{i-u+m-1/2} - x_{i-u+l-1/2}}. \]  

(B.16)
Note that
\[ \sum_{m=0}^{r} \prod_{\substack{l=0 \atop l \neq m}}^{r} \frac{x - x_{i-u+l-\frac{1}{2}}}{x_{i-u+m-\frac{1}{2}} - x_{i-u+l-\frac{1}{2}}} = 1, \]  
which can be proved heuristically by considering the interpolation of a constant function.

To simplify the algebra, \( V(x_{i-u-\frac{1}{2}}) \) is subtracted from Eq. (B.16).

\[ P(x) - V(x_{i-u-\frac{1}{2}}) = \sum_{m=1}^{r} \left( V(x_{i-u+m-\frac{1}{2}}) - V(x_{i-u-\frac{1}{2}}) \right) \prod_{\substack{l=0 \atop l \neq m}}^{r} \frac{x - x_{i-u+l-\frac{1}{2}}}{x_{i-u+m-\frac{1}{2}} - x_{i-u+l-\frac{1}{2}}}. \]  

Using the cell averaged nature of the data,
\[ V(x_{i-u+m-\frac{1}{2}}) - V(x_{i-u-\frac{1}{2}}) = \sum_{j=0}^{m-1} v_{i-u+j} \Delta x_{i-u+j}. \]  

Before the derivative of Eq. (B.18) is taken, note that
\[ \frac{d}{dx} \left[ \prod_{l=0}^{r} (x - x_{i+u+\frac{1}{2}}) \right] = \sum_{q=0}^{r} \prod_{\substack{l=0 \atop l \neq q}}^{r} (x - x_{i+u+q-\frac{1}{2}}). \]  

Substituting Eq. (B.19) into Eq. (B.18) and taking the x-derivative gives the interpolation polynomial, \( p(x) \):
\[ p(x) = \sum_{m=1}^{r} \sum_{j=0}^{m-1} v_{i-u+j} \Delta x_{i-u+j} \left( \sum_{\substack{l=0 \atop l \neq m}}^{r} \prod_{q=0}^{r} (x - x_{i-u+q-\frac{1}{2}}) \right) \left( \prod_{\substack{l=0 \atop l \neq m}}^{r} (x_{i-u+m-\frac{1}{2}} - x_{i-u+l-\frac{1}{2}}) \right). \]
To interpolate the solution data at the cell edge at \( i + \frac{1}{2} \), \( x = x_{i+\frac{1}{2}} \) is simply substituted into Eq. (B.21) producing:

\[
v_{i+\frac{1}{2}} = p(x_{i+\frac{1}{2}}) = \sum_{m=1}^{k} \sum_{j=0}^{m-1} v_{i-u+j} \Delta x_{i-u+j} \left( \sum_{l=0}^{k} \prod_{q=0}^{k} \frac{(x_{i+\frac{1}{2}} - x_{i-u+q-\frac{1}{2}})}{l \neq m \quad q \neq l, m} \right) . \tag{B.22}
\]

If the grid is uniform, we have:

\[
v_{i+\frac{1}{2}} = \sum_{m=1}^{r} \sum_{j=0}^{m-1} v_{i-u+j} \left( \sum_{l=0}^{r} \prod_{q=0}^{r} \frac{(u - q + 1)}{l \neq m \quad q \neq l, m} \right) \frac{1}{\prod (m - l)} . \tag{B.23}
\]

Switching the order of the outside sums gives a form where the coefficients of Eq. (B.15) are readily available:

\[
v_{i+\frac{1}{2}} = \sum_{j=0}^{r-1} \sum_{m=j+1}^{r} \left[ \left( \sum_{l=0}^{r} \prod_{q=0}^{r} \frac{(u - q + 1)}{l \neq m \quad q \neq l, m} \right) \frac{1}{\prod (m - l)} \right] v_{i-u+j} . \tag{B.24}
\]

The coefficients in Eq. (B.15) are finally given by:

\[
\alpha_j^r = \sum_{m=j+1}^{r} \left( \sum_{l=0}^{r} \prod_{q=0}^{r} \frac{(u - q + 1)}{l \neq m \quad q \neq l, m} \right) \frac{1}{\prod (m - l)} . \tag{B.25}
\]
For example, applying Eq. (B.24) to the stencil shown in Figure B.1 produces:

$$v_{i+\frac{1}{2}} = \frac{1}{12}v_{i-2} - \frac{5}{12}v_{i-1} + \frac{13}{12}v_i + \frac{1}{4}v_{i+1}. \quad \text{(B.26)}$$

Due to the integration of the data to form the primitive, the above interpolation procedure is technically valid only for the finite volume method. However, in this work the finite difference method is used. Shu [230] states that the formulas derived using this procedure will work for the finite difference method only if the grid is uniform.

Notice from Figure B.1 that four different four-point stencils could have been chosen to perform the interpolation at $x_{i+\frac{1}{2}}$ that contain at least one upstream point, as shown in Figure B.2.

The idea of Essentially Non-Oscillatory schemes (ENO) developed by Harten et al. [235] is to use the best of all available interpolation stencils that minimizes the Gibbs phenomenon near discontinuities given an $r^{th}$ order accurate interpolation. To increase accuracy in smooth regions, Liu et al. [236] extended ENO by summing the weighted interpolations from all of the available stencils and developed WENO. Using the interpolated values from all valid stencils provides a $2r - 1$ order accurate interpolation in regions where the solution is smooth. In the presence of a discontinuity, stencils that produce unacceptable oscillations must be weighted to zero; reproducing the ENO scheme with order of accuracy $r$ in the worst case. The final
interpolation for the WENO scheme is given by:

\[ v_{i+\frac{1}{2}} = \sum_{k=0}^{r-1} \omega^r_k v^r_{k;i+\frac{1}{2}}, \]  

where \( k \) refers to the stencil number \( (k = 0, 1, \cdots, r-1) \), \( r \) is the number of data points used in each stencil, and \( \omega^r_k \) is the weighting factor of the \( k^{th} \) stencil with order \( r \). The weights are constructed by:

\[ \omega^r_k = \frac{\alpha^r_k}{\sum_{j=1}^{r-1} \alpha^r_j}, \]  

where

\[ \alpha^r_k = \frac{C^r_k}{(IS^r_k + \epsilon)^p}. \]  

The \( C^r_k \) terms are known as the optimal weights, \( IS^r_k \) is the smoothness measure of the stencil, \( \epsilon \) is a small parameter \( (10^{-10} \) in this work) to avoid division by zero, and \( p \) was found by Liu et al. [236] to work best at a value of \( p = 2 \). The calculation of the optimal weights will not be shown in this document, see Liu et al. [236] or Jiang and Shu [237] for more details.

The design of the smoothness indicators has changed considerably from the initial inception of WENO. The most widely used indicators are those from Liu et al. [236], which are defined by:

\[ IS^r_k = \sum_{l=1}^{r-1} \Delta x^{2l-1} \left( \frac{\partial^l p^r_k(x)}{\partial x^l} \right)^2 dx. \]  

The calculation of the smoothness indicators is fairly complex and will not be presented here, see [230, 237] for more details. Other methods for evaluating the smoothness indicators and the stencil weights have been developed [238, 239]. Most of these different methods have not been applied to the very high order schemes and are not considered for use in this work.

If the solution data is known to be smooth (such as most incompressible laminar flows) all of the weights will be equal and the interpolated variable can be calculated directly from the optimal coefficients:

\[ v_{i+\frac{1}{2}} = \sum_{k=0}^{r-1} C^r_k v^r_{k;i+\frac{1}{2}}, \]  

producing the linear-WENO (LWENO) scheme.

In an effort to reduce the dissipation of WENO schemes, Martín et al. [88] developed a revised WENO scheme. They noticed that the original WENO schemes throw out the most
downwind candidate stencil that contains the cell edge but not any upstream grid points. By adding that stencil and recalculating the optimum candidate stencil weights to minimize the dissipation rather than maximizing the formal order of convergence, WENO schemes that retained the same formal order of accuracy as the original version with significantly reduced dissipation were developed. The lower dissipation WENO scheme is called symmetric bandwidth-optimized WENO or WENO-SymBO. They also recommend using \( p = 1 \) in Eq. (B.29) rather than the usual value of \( p = 2 \) when using WENO-SymBO for reduced dissipation.

### B.3.2 Summary of WENO Coefficients

In this section the coefficients and smoothness measures for the WENO3, WENO5, WENO5-SymBO, WENO7, WENO7-SymBO, and WENO9 (i.e., \( r = 2, 3, 4, \) and \( 5 \), respectively) will be presented. To recap, the important equations from the previous section will be given first. The interpolation of a variable at \( x_{i+\frac{1}{2}} \) from the left side, \( v_{L,i+1/2} \) is given by:

\[
v_{L,i+\frac{1}{2}} = \sum_{k=0}^{r-1} \omega_k v_{k; i+\frac{1}{2}}^r.
\]  

(B.32)

The interpolation, \( v_{k;i+\frac{1}{2}}^r \), on stencil \( k \) from the left is:

\[
v_{k;i+\frac{1}{2}}^r = \sum_{j=0}^{r-1} \alpha_k^r v_{i-r+k+j+1} \quad k = 0, 1, \cdots, r - 1,
\]  

(B.33)

and the weighting functions are

\[
\omega_k^r = \frac{\alpha_k^r}{\sum_{j=0}^{r-1} \alpha_j^r},
\]  

(B.34)

where

\[
\alpha_k^r = \frac{C_k^r}{(IS_k^r + \epsilon)^p}.
\]  

(B.35)

The equations presented in the following section assume that the interpolation is from the left.
Table B.1: Reconstruction coefficients for WENO3.

<table>
<thead>
<tr>
<th>$a^2_{k,i}$</th>
<th>$k = 0$</th>
<th>$k = 1$</th>
<th>$C^2_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 0$</td>
<td>$-1/2$</td>
<td>$3/2$</td>
<td>$1/3$</td>
</tr>
<tr>
<td>$i = 1$</td>
<td>$1/2$</td>
<td>$1/2$</td>
<td>$2/3$</td>
</tr>
</tbody>
</table>

Table B.2: Reconstruction coefficients for WENO5 and WENO5-SymBO.

<table>
<thead>
<tr>
<th>$a^3_{k,i}$</th>
<th>$k = 0$</th>
<th>$k = 1$</th>
<th>$k = 2$</th>
<th>$C^3_i$</th>
<th>$C^3_{i_{\text{SymBO}}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 0$</td>
<td>$1/3$</td>
<td>$-7/6$</td>
<td>$11/6$</td>
<td>$1/10$</td>
<td>$0.094647545896$</td>
</tr>
<tr>
<td>$i = 1$</td>
<td>$-1/6$</td>
<td>$5/6$</td>
<td>$1/3$</td>
<td>$6/10$</td>
<td>$0.428074212384$</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$1/3$</td>
<td>$5/6$</td>
<td>$-1/6$</td>
<td>$3/10$</td>
<td>$0.408289331408$</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$11/6$</td>
<td>$-7/6$</td>
<td>$1/3$</td>
<td>NA</td>
<td>$0.068988910311$</td>
</tr>
</tbody>
</table>

B.3.3 Third-Order WENO ($r = 2$)

The coefficients needed to use the WENO3 scheme ($r = 3$) are given in Table B.1. All of the smoothness measures are given below.

\[
IS^2_0 = (v_i - v_{i-1})^2 \\
IS^2_1 = (v_{i+1} - v_i)^2
\]

B.3.4 Fifth-Order WENO ($r = 3$)

The coefficients needed for the WENO5 scheme ($r = 3$) are given in Table B.2. All of the smoothness measures are given below. Note that $IS^3_3$ is only needed for WENO schemes that use the last stencil such as WENO5-SymBO.

\[
IS^3_0 = \frac{13}{12} (v_{i-2} - 2v_{i-1} + v_i)^2 + \frac{1}{4} (v_{i-2} - 4v_{i-1} + 3v_i)^2 \\
IS^3_1 = \frac{13}{12} (v_{i-1} - 2v_i + v_{i+1})^2 + \frac{1}{4} (v_{i-1} - v_{i+1})^2 \\
IS^3_2 = \frac{13}{12} (v_i - 2v_{i+1} + v_{i+2})^2 + \frac{1}{4} (3v_i - 4v_{i+1} + v_{i+2})^2
\]
Table B.3: Reconstruction coefficients for WENO7 and WENO7-SymBO.

<table>
<thead>
<tr>
<th>$a^4_{k,i}$</th>
<th>$k = 0$</th>
<th>$k = 1$</th>
<th>$k = 2$</th>
<th>$k = 3$</th>
<th>$C^4_i$</th>
<th>$C^4_{i,\text{SymBO}}$</th>
</tr>
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<tbody>
<tr>
<td>$i = 0$</td>
<td>$-1/4$</td>
<td>$13/12$</td>
<td>$-23/12$</td>
<td>$25/12$</td>
<td>$1/35$</td>
<td>0.040195483373</td>
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<tr>
<td>$i = 1$</td>
<td>$1/12$</td>
<td>$-5/12$</td>
<td>$13/12$</td>
<td>$1/4$</td>
<td>$12/35$</td>
<td>0.249380000671</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>$-1/12$</td>
<td>$7/12$</td>
<td>$7/12$</td>
<td>$-1/12$</td>
<td>$18/35$</td>
<td>0.480268625626</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>$1/4$</td>
<td>$13/12$</td>
<td>$-5/12$</td>
<td>$1/12$</td>
<td>$4/35$</td>
<td>0.200977547673</td>
</tr>
<tr>
<td>$i = 4$</td>
<td>$25/12$</td>
<td>$-23/12$</td>
<td>$13/12$</td>
<td>$-1/4$</td>
<td>NA</td>
<td>0.029178342658</td>
</tr>
</tbody>
</table>

\[
IS^3_3 = \frac{13}{12} (v_{i+1} - 2v_{i+2} + v_{i+3})^2 + \frac{1}{4} (-5v_{i+1} + 8v_{i+2} - 3v_{i+3})^2
\]

### B.3.5 Seventh-Order WENO$(r = 4)$

The coefficients needed to use the WENO7 scheme $(r = 4)$ are given in Table B.3. All of the smoothness measures are given below. Note that $IS^4_1$ is only needed for WENO schemes that use the last stencil such as WENO7-SymBO.

\[
IS^4_0 = \frac{1}{36} \left( -2v_{i-3} + 9v_{i-2} - 18v_{i-1} + 11v_i \right)^2 + \frac{13}{12} \left( -v_{i-3} + 4v_{i-2} - 5v_{i-1} + 2v_i \right)^2 + \frac{781}{720} \left( -v_{i-3} + 3v_{i-2} - 3v_{i-1} + v_i \right)^2
\]

\[
IS^4_1 = \frac{1}{36} \left( v_{i-2} - 6v_{i-1} + 3v_i + 2v_{i+1} \right)^2 + \frac{13}{12} \left( v_{i-1} - 2v_i + v_{i+1} \right)^2 + \frac{781}{720} \left( -v_{i-2} + 3v_{i-1} - 3v_i + v_{i+1} \right)^2
\]

\[
IS^4_2 = \frac{1}{36} \left( -2v_{i-1} - 3v_i + 6v_{i+1} - v_{i+2} \right)^2 + \frac{13}{12} \left( v_{i-1} - 2v_i + v_{i+1} \right)^2 + \frac{781}{720} \left( -v_{i-1} + 3v_i - 3v_{i+1} + v_{i+2} \right)^2
\]

\[
IS^4_3 = \frac{1}{36} \left( -11v_i + 18v_{i+1} - 9v_{i+2} + 2v_{i+3} \right)^2 + \frac{13}{12} \left( 2v_i - 5v_{i+1} + 4v_{i+2} - v_{i+3} \right)^2 + \frac{781}{720} \left( -v_i + 3v_{i+1} - 3v_{i+2} + v_{i+3} \right)^2
\]

\[
IS^4_4 = \frac{1}{36} \left( -26v_{i+1} + 57v_{i+2} - 42v_{i+3} + 11v_{i+4} \right)^2 + \frac{13}{12} \left( 3v_{i+1} - 8v_{i+2} + 7v_{i+3} - 2v_{i+4} \right)^2 + \frac{781}{720} \left( -v_{i+1} + 3v_{i+2} - 3v_{i+3} + v_{i+4} \right)^2
\]
Table B.4: Reconstruction coefficients for WENO9.

<table>
<thead>
<tr>
<th>$a_{k,i}^5$</th>
<th>$k = 0$</th>
<th>$k = 1$</th>
<th>$k = 2$</th>
<th>$k = 3$</th>
<th>$k = 4$</th>
<th>$C_i^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i = 0$</td>
<td>1/5</td>
<td>-21/20</td>
<td>137/60</td>
<td>-163/60</td>
<td>137/60</td>
<td>1/126</td>
</tr>
<tr>
<td>$i = 1$</td>
<td>-1/20</td>
<td>17/60</td>
<td>-43/60</td>
<td>77/60</td>
<td>1/5</td>
<td>10/63</td>
</tr>
<tr>
<td>$i = 2$</td>
<td>1/60</td>
<td>-13/60</td>
<td>47/60</td>
<td>9/20</td>
<td>-1/20</td>
<td>10/21</td>
</tr>
<tr>
<td>$i = 3$</td>
<td>-1/20</td>
<td>9/20</td>
<td>47/60</td>
<td>-13/60</td>
<td>1/60</td>
<td>20/63</td>
</tr>
<tr>
<td>$i = 4$</td>
<td>1/5</td>
<td>77/60</td>
<td>-43/60</td>
<td>17/60</td>
<td>-1/20</td>
<td>5/126</td>
</tr>
</tbody>
</table>

B.3.6 Ninth-Order WENO ($r = 5$)

The coefficients needed to use the WENO9 scheme ($r = 5$) are given in Table B.4. All of the smoothness measures are given below.

\[ IS_0^5 = v_{i-4} (22658v_{i-4} - 208501v_{i-3} + 364863v_{i-2} - 288007v_{i-1} + 86329v_i) \]
\[ + v_{i-3} (482963v_{i-3} - 1704396v_{i-2} + 1358458v_{i-1} - 411487v_i) \]
\[ + v_{i-2} (1521393v_{i-2} - 2462076v_{i-1} + 758823v_i) \]
\[ + v_{i-1} (1020563v_{i-1} - 649501v_i) + 107918v_i^2 \]
\[ IS_1^5 = v_{i-3} (6908v_{i-3} - 60871v_{i-2} + 99213v_{i-1} - 70237v_i + 18079v_{i+1}) \]
\[ + v_{i-2} (138563v_{i-2} - 464976v_{i-1} + 337018v_i - 88297v_{i+1}) \]
\[ + v_{i-1} (406293v_{i-1} - 611976v_i + 165153v_{i+1}) \]
\[ + v_i (242723v_i - 140251v_{i+1}) + 22658v_{i+1}^2 \]
\[ IS_2^5 = v_{i-2} (6908v_{i-2} - 51001v_{i-1} + 67923v_i - 38947v_{i+1} + 8209v_{i+2}) \]
\[ + v_{i-1} (104963v_{i-1} - 299076v_i + 179098v_{i+1} - 38947v_{i+2}) \]
\[ + v_i (231153v_i - 299076v_{i+1} + 67923v_{i+2}) \]
\[ + v_{i+1} (104963v_{i+1} - 51001v_{i+2}) + 6908v_{i+2}^2 \]
\[ IS_3^5 = v_{i-1} (22658v_{i-1} - 140251v_i + 165153v_{i+1} - 88297v_{i+2} + 18079v_{i+3}) \]
\[ + v_i (242723v_i - 611976v_{i+1} + 337018v_{i+2} - 70237v_{i+3}) \]
\[ + v_{i+1} (406293v_{i+1} - 464976v_{i+2} + 99213v_{i+3}) \]
\[ + v_{i+2} (138563v_{i+2} - 60871v_{i+3}) + 6908v_{i+3}^2 \]
\[ IS_4^5 = v_i (107918v_i - 649501v_{i+1} + 758823v_{i+2} - 411487v_{i+3} + 86329v_{i+4}) + v_{i+1} (1020563v_{i+1} - 246076v_{i+2} + 1358458v_{i+3} - 288007v_{i+4}) + v_{i+2} (1521393v_{i+2} - 1704396v_{i+3} + 364863v_{i+4}) + v_{i+3} (482963v_{i+3} - 208501v_{i+4}) + 22658v_{i+4} \]

**B.3.7 LWENO Schemes**

In cases where the flow features are smooth, the so-called LWENO schemes can be used. The LWENO schemes are simply what the WENO schemes reduce to if all the candidate stencils have the same smoothness coefficients and interpolated value is evaluated using just the optimal stencil coefficients.

\[ v_{L,i+1/2}^2 = \frac{1}{6} v_{i-1} + \frac{5}{6} v_i + \frac{1}{3} v_{i+1} \]  
\[ v_{L,i+1/2}^3 = \frac{1}{10} v_{i-2} - \frac{13}{60} v_{i-1} + \frac{47}{60} v_i + \frac{9}{20} v_{i+1} - \frac{1}{20} v_{i+2} \]  
\[ v_{L,i+1/2}^4 = \frac{5}{84} v_{i-2} - \frac{101}{420} v_{i-1} + \frac{319}{420} v_i + \frac{107}{210} v_{i+1} - \frac{19}{210} v_{i+2} + \frac{1}{105} v_{i+3} \]  
\[ v_{L,i+1/2}^5 = \frac{1}{630} v_{i-4} - \frac{41}{2520} v_{i-3} + \frac{199}{2520} v_{i-2} - \frac{641}{2520} v_{i-1} + \frac{1879}{2520} v_i - \frac{275}{504} v_{i+1} + \frac{61}{504} v_{i+2} + \frac{11}{504} v_{i+3} - \frac{1}{504} v_{i+4} \]

For WENO-SymBO schemes, the LWENO interpolations become

\[ v_{L,i+1/2}^{3,SymBO} = 0.03154918196533333v_{i-2} - 0.18176783894266668v_{i-1} + 0.666345454932v_i + 0.6094121825381668v_{i+1} - 0.60635283930833335v_{i+2} + 0.022996303437v_{i+3} \]
Taylor, Wu, and Martín [202] noticed that the WENO schemes, including the WENO-SymBO scheme [88], are too dissipative for compressible turbulent direct numerical simulation (DNS) or large eddy simulation (LES) calculations. They determined that the cause for the excessive dissipation is that WENO schemes not being very aggressive in relatively smooth regions and tend to over-adapt the candidate stencils. To obtain a more aggressive stencil they proposed forcing the LWENO scheme if the smoothness measures on all of the stencils are sufficiently close or the total variation ($TV$) is sufficiently close on all the candidate stencils. The total variation of variable $v$ on stencil $k$ containing $r$ grid points is defined by:

$$TV_k(v) = \sum_{j=1}^{r-1} |v_{i-r+k+j+1} - v_{i-r+k+j}|.$$  \hspace{1cm} (B.42)

The closeness of the smoothness measures, $R_{IS}$, and the total variation measures, $R_{TV}$, are defined by:

$$R_{IS} = \frac{\max IS_k}{\epsilon + \min IS_k},$$

$$R_{TV} = \frac{\max TV_k}{\epsilon + \min TV_k}.$$  \hspace{1cm} (B.43)

The selection between WENO and LWENO is performed by:

$$\text{Method} = \begin{cases} 
\text{LWENO} & \text{if } R_{IS} < \alpha_{IS} \text{ or } (R_{TV} < \alpha_{TV} \text{ and } \max (TV_k) < \beta_{TV}) \\
\text{WENO} & \text{otherwise,}
\end{cases}$$

(B.44)

where $\alpha_{IS} = 10$, $\alpha_{TV} = 5$ for WENO5 and WENO5-SymBO, $\alpha_{TV} = 4$ for WENO7 and WENO7-SymBO, and $\beta_{TV} = 0.2$ [202, 240]. This method can be used to reduce the dissipation of either WENO or WENO-SymBO schemes.
B.5 Monotonicity Preserving WENO

WENO schemes perform well at suppressing the Gibbs phenomenon near discontinuities; however, they do not perfectly preserve monotonicity when the smoothness measures are terrible for all candidate stencils. A numerical scheme for hyperbolic conservation laws is called monotonicity-preserving (MP) if the solution that is initially monotonic remains monotonic in the absence of source terms [114]. Suresh and Huynh [136] developed a 5th-order MP scheme, that forces the interpolated variable to be within physical bounds. The oscillations in the solution are distinguished from physical extrema by analyzing the curvature of the solution data in characteristic form. Balsara and Shu [119] adopted this method to apply bounds to the WENO-interpolated variables, and called their scheme MPWENO.

The procedure of [136] is summarized below for interpolation of a variable from the left. First, the minmod and median functions are defined:

\[
\text{minmod}(x_1, x_2, \cdots, x_n) = \frac{1}{2^n-1} \min(|x_1|, |x_2|, \cdots, |x_n|) \prod_{j=2}^{n} [\text{sgn}(x_1) + \text{sgn}(x_j)], \tag{B.45}
\]

\[
\text{median}(x_1, x_2, x_3) = x_1 + \text{minmod}(x_2 - x_1, x_3 - x_1). \tag{B.46}
\]

The minmod function clips local extrema by simply returning the minimum argument if all arguments are positive, the maximum argument if all arguments are negative, and zero otherwise.

The local cell curvature, \(d_i\), is defined based on the second derivative calculated with second-order central difference:

\[
d_i = v_{i+1} - 2v_i + v_{i-1}. \tag{B.47}
\]

Now the upper limit of the interpolated variable, \(v_{i+\frac{1}{2}}^U\), the interpolated value with allowance for large curvatures, \(v_{i+\frac{1}{2}}^C\), and median of the limits, \(v_{i+\frac{1}{2}}^{MD}\), are defined by:

\[
v_{i+\frac{1}{2}}^U = v_i + \alpha(v_i - v_{i-1}), \tag{B.48}
\]

\[
v_{i+\frac{1}{2}}^C = v_i + \frac{1}{2}(v_i - v_{i-1}) + \frac{\beta}{3} d_{j-\frac{1}{2}}^C, \tag{B.49}
\]

\[
v_{i+\frac{1}{2}}^{MD} = \frac{1}{2} \left( v_i + v_{i+1} - d_{j+\frac{1}{2}}^{MD} \right), \tag{B.50}
\]
where $\alpha$ and $\beta$ are parameters to be set by the user. The theory developed by Suresh and Huynh [136] states that:

$$CFL \leq \frac{1}{1 + \alpha},$$

although Balsara and Shu [119] found that it was safe to use a CFL number of 0.6 when $\alpha = 2$ for most problems. There is no theory to help in setting the parameter, $\beta$; a value of 4 was found to be sufficient in most test cases [119].

Using the above definition, limits on the minimum and the maximum of the interpolated variable are:

$$v_{i+\frac{1}{2}}^{\min} = \max \left[ \min \left( v_i, v_{i+1}, v_{i+\frac{1}{2}}^{MD} \right), \min \left( v_i, v_{L,i+\frac{1}{2}}, v_{i+\frac{1}{2}}^{C} \right) \right],$$  \hspace{1cm} (B.51)

$$v_{i+\frac{1}{2}}^{\max} = \min \left[ \max \left( v_i, v_{i+1}, v_{i+\frac{1}{2}}^{MD} \right), \max \left( v_i, v_{L,i+\frac{1}{2}}, v_{i+\frac{1}{2}}^{C} \right) \right].$$  \hspace{1cm} (B.52)

The MPWENO interpolated variable, $(v_{i+\frac{1}{2}}^{\text{MPWENO}})$, is taken as:

$$v_{i+\frac{1}{2}}^{\text{MPWENO}} = \text{median} \left( v_{i+\frac{1}{2}}^{\text{WENO}}, v_{i+\frac{1}{2}}^{\min}, v_{i+\frac{1}{2}}^{\max} \right).$$  \hspace{1cm} (B.53)

Several methods exist to evaluate the large and median curvatures; Balsara and Shu [119] used one of three:

$$d_{i+\frac{1}{2}}^{MM} = \text{minmod} \left( d_i, d_{i+1} \right),$$  \hspace{1cm} (B.54)

$$d_{i+\frac{1}{2}}^{M4} = \text{minmod} \left( 4d_i - d_{i+1}, 4d_{i+1} - d_i, d_i, d_{i+1} \right),$$  \hspace{1cm} (B.55)

$$d_{i+\frac{1}{2}}^{M4X} = \text{minmod} \left( 4d_i - d_{i+1}, 4d_{i+1} - d_i, d_i, d_{i+1}, d_{i-1}, d_{i+2} \right).$$  \hspace{1cm} (B.56)

### B.6 Edge Interpolation from the Right

When interpolating from the right to estimate $u_{R,i+1/2}$, the reconstruction schemes need to be slightly modified using stencil symmetry. The equations for $u_{R,i+1/2}$ are formed by shifting the stencil to the right by one and then permuting the cell indexes in the equations for $u_{L,i+1/2}$. The optimal coefficients and reconstruction coefficients, themselves are unchanged using this mapping. The interpolation formulae for MUSCL, WENO, and MPWENO can be used directly if the cell mapping shown in Table B.5 is applied.
Table B.5: Cell index mapping from left edge interpolation to right edge interpolation.

<table>
<thead>
<tr>
<th>$v_L$ grid point</th>
<th>$i-3$</th>
<th>$i-2$</th>
<th>$i-1$</th>
<th>$i$</th>
<th>$i+1$</th>
<th>$i+2$</th>
<th>$i+3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_R$ grid point</td>
<td>$i+4$</td>
<td>$i+3$</td>
<td>$i+2$</td>
<td>$i+1$</td>
<td>$i$</td>
<td>$i-1$</td>
<td>$i-2$</td>
</tr>
</tbody>
</table>

Applying the mapping to the smoothness indicator for the $k = 2$ stencil of WENO5 gives:

$$IS_2^3 = \frac{13}{12} (v_{i+1} - 2v_i + v_{i-1})^2 + \frac{1}{4} (3v_{i+1} - 4v_{i-1} + v_{i-2})^2.$$  \hspace{1cm} (B.57)

Note that the mapping shown in Table B.5 also applies the MUSCL scheme discussed above; however, the mapping must be applied to the definition of the slope ratio, Eq. (B.4), rather than the slope ratio itself.

B.7 Comparison of Interpolation Methods

The accuracy of the edge interpolation schemes were compared by solving the scalar wave problem:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \quad -1 < x < 1,$$

$$u(x, 0) = u_0(x),$$ \hspace{1cm} (B.58)

with periodic boundary conditions. The initial profile is:

$$u_0 = \begin{cases} 
\frac{1}{6}[G(x, \beta, z - \delta) + G(x, \beta, z + \delta) + 4G(x, \beta, z)] & -0.8 \leq x \leq -0.6 \\
1 & -0.4 \leq x \leq -0.2 \\
1 - \left| 10(x - 0.1) \right| & 0.0 \leq x \leq 0.2 \\
\frac{1}{6}[F(x, \alpha, a - \delta) + G(x, \alpha, a + \delta) + 4F(x, \alpha, a)] & 0.4 \leq x \leq 0.6 \\
0 & \text{otherwise,}
\end{cases}$$ \hspace{1cm} (B.59)
Figure B.3: Solution profile to Eq. (B.58) after ten traversals using a variety of MPWENO schemes with the M4X curvature limiter.

This problem was solved using a variety of interpolation methods given in this appendix. The fluxes were formed by interpolation in the upwind direction and were integrated in time using the RK3 scheme with a Courant number of 0.3 unless otherwise noted. The mesh in all cases consisted of 400 cells. The solution after ten traversals around the domain using MPWENO schemes and first-order upwind are shown in Figure B.3. It is clear that all of the MPWENO schemes do a perform relatively well while first-order interpolation completely destroys the profile. The third-order MPWENO (MPWENO3) scheme exhibit quite a bit dissipation and destroys the delicate features of the advected shapes while MPWENO5 and MPWENO9 do an excellent job of maintaining the integrity of the shapes.

The solution using the MUSCL interpolation with a variety of slope limiters and MPWENO3 is shown in Figure B.4. Of all the third-order MUSCL schemes, the MLP3 limiter has the best performance since it maintains the sharp features of initial profile without dis-
torting the shapes. The superbee limiter does an extremely good on the square wave (better then MPWENO9), but this comes at the cost of being overly compressive. Compressive limiters, such as superbee, can actually sharpen smooth features, producing stair-case like features, which is observed on the half-ellipse (rightmost) shape. MPWENO3 is one of the worst performers of the third order schemes.

A comparison of the results using fifth-order MUSCL (MPL5) and MPWENO5 on the square wave and half-ellipse are shown in Figure B.5. MLP5 and MPWENO exhibit very similar performance, with the exception that MUSCL5 exhibits some clipping (i.e., the flattening of the half-ellipse). It has been noted that WENO5 exhibits small, but not destructive, instabilities when the CFL number is too high. These small instabilities are observed in the square wave of Figure B.5a when the CFL number was increased from 0.3 to 0.8. These small instabilities do not occur with MUSCL using the MLP5 limiter. In terms of computational efficiency to reach the same calculation time, MUSCL5 is 4.7 times faster than MPWENO5 if the same CFL number is used. The large discrepancy of the execution times is due to the large expense of evaluating the smoothness coefficients for the WENO candidate stencils. If the different CFL numbers are taken into account, MUSCL5 is 12.5 times faster than MPWENO5 with roughly the same accuracy.
Figure B.5: Comparison of MLP5 and MPWENO5 schemes on the advection test: (a) close-up of the square wave and (b) close-up of the half-ellipse.
VERIFICATION TESTS

This chapter provides detailed information on many of the verification problems that were used to ensure that the developed software is working properly. Problems with exact, analytical solutions were used wherever possible. Solutions using the internationally accepted Chemkin code [206] were used in place of analytical solutions when verifying fully non-linear convection, diffusion, and reaction problems. Certain verification tests were compared against literature values.

C.1 Single Component Gaseous Riemann Problems

In this section the performance of the AUSM$^+$, Rusanov, and the characteristic-based Local Lax-Friedrichs flux vector splitting (denoted LLF FVS) are compared against several Riemann problems. The problems are initialized by setting $Q = (\rho, p, u)$ to $Q_L$ to the left of a diaphragm located at $x = x_{\text{diaphragm}}$ and $Q_R$ to the right of the diaphragm. The problems include the shock tube problem, the colliding shock problem, and the moving contact problems. In all cases the domain is one meter long and the M4X monotonicity-preserving method was used for MPWENO interpolation. Time advancement was performed using the third-order strong-stability preserving Runge-Kutta (RK3).
Figure C.1: Comparison of (a) flux evaluation methods using 300 cells and (b) grid convergence using LLF FVS with MPWENO9 interpolation on the shock tube problem.

C.1.1 Shock Tube Problem

In initial conditions for this problem are given by $Q_L = (13 \text{ kg/m}^3, 10 \text{ atm}, 0)$ and $Q_R = (1.3 \text{ kg/m}^3, 1 \text{ atm}, 0)$. The diaphragm is located at 0.4 m. The solution is advanced to a time of 1 ms using the SSP-RK3 scheme with a CFL number of 0.3. Figure C.1a shows the performance of the flux evaluation schemes with a uniform grid and Figure C.1b shows the effect of grid resolution using the LLF FVS scheme with MPWENO9 interpolation. It is clear that all of the methods do a good job of calculating the rarefaction wave and the shock, although the AUSM$^+$ and the Rusanov flux exhibits a slight oscillation at the tail of the rarefaction wave when MPWENO9 is used. Where the schemes differ the most is at the front of the contact surface. Both the AUSM$^+$ and the Rusanov fluxes exhibit slight undershoots at the head of the contact surface with using MPWENO9, while the LLF FVS remains monotonic. If this was a multi-component shock tube problem, these undershoots could cause negative mass fractions.
C.1.2 Colliding Shock Problem

Some high-order methods produce short wavelength oscillations when two shocks collide; the colliding shock problem tests how well schemes perform when shocks collide or reflect off walls. The initial conditions for this problem are $Q_L = (1.3 \text{ kg/m}^3, 1 \text{ atm}, 500 \text{ m/s})$ and $Q_R = (1.3 \text{ kg/m}^3, 1 \text{ atm}, -500 \text{ m/s})$ with the diaphragm located at 0.5 m. Variable interpolation was performed using MPWENO5. The calculated results at a time of 0.4 ms are shown in Figure C.2. Only the LLF FVS method was oscillation free. Both AUSM$^+$ and the Rusanov flux exhibited short wavelength oscillations; although the oscillation of AUSM$^+$ are not quite as severe. Note that almost all flux schemes exhibit a small temperature spike at the location where two shocks collide which is not remedied with grid refinement [241].

C.1.3 Moving Contact Problem

The initial conditions for this problem are $Q_L = (1.3 \text{ kg/m}^3, 1 \text{ atm}, 100 \text{ m/s})$ and $Q_R = (13 \text{ kg/m}^3, 1 \text{ atm}, 100 \text{ m/s})$, which sets up a density wave that should passively advect with the fluid velocity. Unfortunately in the presence of a contact surface many schemes will exhibit oscillations in velocity and pressure even though they were initially uniform. Figure C.3 shows the computed velocity profile after 2 ms (variable interpolation was performed using WENO5). In addition to comparing the flux evaluation, the effects of which variables were
interpolated (conserved or primitive) was examined with the AUSM$^+$ scheme. The only two schemes that maintained a uniform velocity field were LLF FVS and AUSM$^+$ interpolated with primitive variables ($p$, $u$, $T$). It is interesting to note that even though AUSM$^+$ with primitive variable interpolation performed extremely well, AUSM$^+$ with conserved variable interpolation had the worst performance showing the most severe oscillations. The reason for the difference when interpolating primitive or conserved variables is that the primitive variables $p$ and $u$ are both constant in this problem, while none of the conserved variables are constant, leading to slight differences in the nonlinear edge interpolation process and the AUSM$^+$-up flux calculation.

C.1.4 Cylindrical and Spherical Riemann Problems

The two-dimensional Euler equations are solved on the unit square with initial conditions consisting of an initially stagnant domain with a high-pressure region inside of a circle of radius $R = 0.4$ m centered at the origin. The initial conditions taken inside and outside of

**Figure C.3:** Comparison of flux evaluation scheme on the calculated velocity profile of moving contact problem.
Symmetry boundary conditions are used on all sides of the domain. The solution is marched in time using a CFL number of 0.3 using MPWENO7 with in conjunction with the AUSM+-up flux to a time of $t = 0.25$ s. Dimensional sweeping was performed using Strang splitting. The spherical problem is identical to the cylindrical with the exception that it is solved in axisymmetric rather than Cartesian coordinates. The mesh in either case used a 100 by 100 grid.

Since there is not an exact solution to these problems, the calculations are compared to reference solutions found in Chapter 17 of Toro [113]. The one-dimensional solution of these problems using 1000 cells was found to be in excellent agreement with the reference solution and thus, will be used in place of an exact solution. The solution to the cylindrical and spherical Riemann problems can be found in Figure C.4. The calculated multi-dimensional results agree quite well with the 1-D solution, in fact the one-dimensional and multi-dimensional calculations using the same number of cells are nearly indistinguishable. Since the solutions

\[ \begin{align*}
\rho_{\text{in}} &= 1.000 & \rho_{\text{out}} &= 0.125 \\
u_{\text{in}} &= 0.000 & u_{\text{out}} &= 0.000 \\
v_{\text{in}} &= 0.000 & v_{\text{out}} &= 0.000 \\
p_{\text{in}} &= 1.000 & p_{\text{out}} &= 0.100.
\end{align*} \]  

(C.1)
to these problems are a function of time and radius (provided that Rayleigh-Taylor instabilities on the contact surface have not formed), the density was sampled at various angles of 0, 30, 45, 60, and 90 degrees to check for any directional bias caused by the directional sweeping. It is clear from Fig C.4 that any directional bias in the calculations is very weak.

### C.2 Constant-Property Advection and Diffusion

This problem tests the advection of a diffusive front consisting of two different gases with identical thermo-physical properties (set up to be those of $H_2$). If the initial pressure, temperature, and velocity are initially uniform in the domain and transmissive boundary conditions are used it is possible to show that 1-D Navier-Stokes equations reduce to:

\[
\frac{\partial \rho}{\partial t} = 0 \quad (C.2)
\]

\[
\frac{\partial u}{\partial t} = 0 \quad (C.3)
\]

\[
\frac{\partial T}{\partial t} = 0 \quad (C.4)
\]

\[
\frac{\partial Y_1}{\partial t} = -u \frac{\partial Y_1}{\partial x} + D \frac{\partial^2 Y_1}{\partial x^2} \quad (C.5)
\]

\[
Y_2 = 1 - Y_1. \quad (C.6)
\]

If the initial condition on $Y_1$ is given by:

\[
Y_1(x, 0) = \begin{cases} 
1 & x \leq x_i \\
0 & x > x_i,
\end{cases} \quad (C.7)
\]

it can be shown that the exact solution to the mass fraction is:

\[
Y_1(x, t) = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{x - x_i - ut}{2\sqrt{Dt}} \right) \right], \quad (C.8)
\]

where \( \text{erf} \) is the Gaussian error function defined as:

\[
\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-s^2} ds.
\]
The governing equations were integrated using Strang splitting, with the hyperbolic portion integrated using RK3 and the parabolic portion integrated using RKC with four stages. The hyperbolic portion was spatially discretized using fifth-order MPWENO-SymBO in conjunction with AUSM\textsuperscript{+}-up. Conservative second-order differencing was used to compute the diffusive fluxes. Shown in Figure C.5 is the solution to the advection diffusion problem. Note that the 1-D Navier-Stokes equations were solved, not the simplified system shown above. Thermal properties were taken to be those of hydrogen at a temperature of 1000 K \( \mathcal{D} = 0.0011 \text{ m}^2/\text{s} \) and atmospheric pressure. The grid spacing was fixed at \( \Delta x = 15 \ \mu\text{m} \) and the diffusive front was allowed to travel a total distance of 2 mm. Different velocities were used to vary the Mach number from \( M = 0.0076 \) to \( M = 7.6 \) with corresponding cell Peclet numbers, \( Pe = u\Delta x/\mathcal{D} \), ranging from 0.272 to 272.

It is clear that the calculated results agree very well with the exact solutions, especially at low Peclet numbers. All advection schemes tend to round off sharp diffusive fronts, which is evident in Figure C.5d. In most cases the additional diffusion produced by the advection scheme is quite small, which the reason that high-order low-dissipation advection schemes are used even though a formal analysis of the grid convergence rate would be second order. If advection schemes of third order or less are used, the rounding effect can be quite severe as shown in Figure C.6.

### C.3 Lid-Driven Cavity

This classical test problem solves the Navier-Stokes equations in a unit box. The boundaries of the box are treated as no-slip walls with the sides and bottom stationary and the top lid moving at a fixed velocity. The Mach number of the lid was fixed at 0.08 to ensure that compressibility effects are negligible. The Reynolds number, \( Re_H = \rho U_{\text{lid}} H/\mu \), of the cavity based on the lid velocity, \( U_{\text{lid}} \), and cavity depth, \( H \), was set to 400 and 1000 for two different cases.

The solution was marched to steady-state at CFL = 0.3 and was spatially discretized using MPWENO7 to interpolate the characteristic variables with the slope limiter applied everywhere at all locations on a 128×128 mesh. RKC was used to integrate the parabolic terms with two stages. The LM adjustment was not applied. Boundary conditions were implemented by reflecting the velocity about the prescribed wall values and using a simple reflection criterion on all other variables. Steady-state, in the classical sense, is difficult to
Figure C.5: Comparison between the exact and calculated solution of the advection diffusion equation after the front has moved a distance of 0, 0.5, 1, 1.5, and 2 mm with (a) $P_{\text{cell}} = 0.272$ and $M = 0.0076$, (b) $P_{\text{cell}} = 2.72$ and $M = 0.076$, (c) $P_{\text{cell}} = 27.2$ and $M = 0.76$, and (d) $P_{\text{cell}} = 272$ and $M = 7.6$. Note that all calculated data points are plotted for (c) and (d) while only every fourth data point is plotted in (a) and (b) for clarity.

achieve using unsteady compressible flow methods at low Mach numbers. Low-amplitude pressure waves form during startup and take an impractical amount of time to fully dissipate using unsteady, low-dissipation methods. In place of a traditional convergence criterion, convergence was considered to be achieved when the calculated velocity fields for 400 consecutive time steps were not noticeably different.

The calculated streamlines and velocity contour plots, shown in Figure C.7, are in excellent agreement with the numerical acoustic relaxation formulation of Nourgaliev et al. [172] and the $\psi - \omega$ formulation Ghia et al. [242]. A comparison between the tabulated data of
Figure C.6: Effect interpolation order-of-accuracy on the advection of a diffusive front, $Pe_{cell} = 118$ and $D = 2.6 \times 10^{-5} \text{ m}^2/\text{s}$.

Figure C.7: Lid driven cavity test; calculated results showing streamlines and $x$-velocity field of the lid driven cavity problem at Reynolds numbers of (a) 400 and (b) 1000.

Ghia et al. and the calculated results from this study is shown in Figure C.8 with very close agreement.
Figure C.8: Lid driven cavity test; comparison between calculated velocity profiles of Ghia et al. [242] and this work: (a) dimensionless x-velocity and (b) dimensionless y-velocity.

C.4 Axisymmetric Couette Flow

In this problem calculates the velocity and temperature profiles in the annular region between concentric tubes. The flow is driven by moving the outer tube at velocity $U$. Viscous dissipation produces a non-monotonic temperature profile in the annular region, which is balanced by a net heat flux out of the tube walls. Since the calculated velocity and temperature fields are one-dimensional in the radial direction, an exact solution can be found for the axial velocity, $u$:

$$u(r) = U \frac{\ln(r/r_i)}{\ln(r_o/r_i)},$$

(C.9)

and the temperature $T$:

$$T(r) = T_i \ln(r/r_o) - T_o \ln(r/r_i) - \frac{U^2 \mu \ln(r/r_i) \ln(r/r_o)}{2 \alpha \ln(r_i/r_o)},$$

(C.10)

where $r_i$ and $r_o$ are the inner and outer radii of the annular region and $T_i$ and $T_o$ are the temperatures of the inner and outer tubes.

The numerical solution to this problem was calculated by marching the single component, constant property Navier-Stokes equations in the two-dimensional axisymmetric coordinate
system to steady state. Even though radial diffusion is the only physical process occurring in Couette flow, the hyperbolic portion of the conservation equations was solved in addition to the parabolic terms. Since the converged flow field is one-dimensional, only five cells were used in the axial direction. The inner and outer radii of the annular region were $r_i = 100 \, \mu m$ and $r_o = 930 \, \mu m$ with $T_i = 293 \, K$ and $T_o = 294 \, K$. The fluid was taken to be air with $\gamma = 1.4$, $\mu = 1.57 \times 10^{-5} \, \text{Pas}$, $C_p = 1006 \, \text{J/kgK}$, and $Pr = 0.708$. The velocity of the outer tube was set to $U = 75.4 \, \text{m/s}$.

The converged velocity and temperature profiles shown in Figure C.9 agree quite well with the exact solution. Since the velocity and temperature profiles are governed by diffusion mechanisms, the overall convergence rate is second order. The success of this test verifies that viscous stresses and viscous dissipation in axisymmetric coordinates are calculated properly. Note that the Cartesian version of this problem was also verified, but is not discussed for the sake of brevity.

C.4.1 Viscous Shock Tube

This problem calculates the interaction between a shock wave and a laminar boundary layer. Initially, a shock and contact wave are sent down a tube by an instant rupture of a diaphragm located at $x = 0.5 \, \text{m}$. Since no-slip and adiabatic boundary conditions are placed on the upper and lower walls of the 2D-planar shock tube, a boundary layer develops behind the
shock wave. Eventually the shock waves reflects off the end wall located at \( x = 1 \) m and interacts with the boundary layer. Since the velocity of the gas in the boundary layer is less than the core flow, the reflected shock wave in the boundary layer region outraces the reflected shock wave in the core flow. The result of this phenomenon is that the shock wave in the boundary layer becomes oblique producing a reduced stagnation pressure in the boundary layer, which causes it to separate, leading to an unsteady turbulent flow. The oblique shock also forms a classical \( \lambda \) shock and triple point, which turns the obliquely-shocked gas back to the parallel direction outside of the boundary layer. Richtmyer-Meshkov and Kelvin-Helmholtz instabilities occur when the reflected shock wave interacts with the contact surface, generating additional vorticity and complicating the flow field structure.

There is not an exact solution to this problem; however, the results from this work can be compared to those of Daru and Tenaud [243] and Kim and Kim [124, 137].

The calculation is performed in a region where no-slip, adiabatic boundary conditions are used on the left, right, and bottom of the domain. A symmetry condition is employed on the upper boundary. The initial conditions on the left and right side of the diaphragm, located at \( x = 0.5 \) m, are:

\[
\begin{align*}
\rho_L &= 1.20 & \rho_R &= 120 \\
p_L &= \rho_L / \gamma & p_R &= \rho_R / \gamma \\
u_L &= 0 & u_R &= 0 \\
v_L &= 0 & v_R &= 0,
\end{align*}
\]

where \( \gamma \) is taken to be 1.4 and the molecular weight is 28.97. The shear viscosity and thermal conductivity are given by:

\[
\mu = \frac{1}{Re}, \quad \lambda = \frac{\mu R}{(\gamma - 1)RePr},
\]

where the Prandtl number, \( Pr \), is 0.73. Note that the reference values for density, velocity, and length are all unity for the definition of the Reynolds number. Spatial discretization was performed using seventh-order WENO-SymBO to interpolate the characteristic variables with the slope limiter applied everywhere. The solution was marched in time using RK2 and a CFL number of 0.3 to a time of \( t = 1 \) s. The rotated Riemann solver was not used in this
The integration of the parabolic operator was performed using RKC with three stages.

The calculated solution at a time of 1 s for $Re = 200$ is shown in Figure C.10 and is presented in a manner that mimics that figures shown in Daru and Tenaud [243] for easy comparison. The results calculated in this work show extremely close agreement with the reference calculations.

### C.5 Constant-Volume Reactor

To verify the source term integrator and the thermodynamic property evaluation, a stoichiometric constant-volume reactor problem of stoichiometric $Al(l)$ and air was setup using the library developed for this work and the results are shown in Figure C.11. The reaction mechanism used for this problem is given in Table 2.1. The liquid aluminum/air mixture was initially at a temperature of 2300 K and a pressure of 1 atm. The temperature increment in the thermodynamic and reaction rate constant tables was $\Delta T = 1$ K. The library was verified by comparing the results from the developed library to the calculated results of the same problem using Chemkin 4.1.1 [206], which is shown in Figure C.12.

It is clear that the calculated results using the developed library compare very well with the Chemkin results, which is a standard and validated tool for gas-phase chemical kinetic calculations, with no more than 0.2% difference between Chemkin and the developed library. The calculated results show that the reaction of $Al/air$ air is very fast and energetic, with the overall event taking around one $\mu s$ to complete.
Figure C.11: Calculated temperature and species mass fraction for the stoichiometric Al/Air constant volume reactor problem (a) in the time range of 1 ns to 10 µs (b) zoomed in to 100 ns to 1 µs.

Figure C.12: Comparison of and percent difference between the calculated (a) temperature and (b) AlO mass fraction profiles using the code developed for this work and Chemkin.
C.6 Liquid Shock Tube Problem

In this section the performance of the hybrid flux evaluation scheme is assessed for the liquid shock tube problem. The parameters for the Tait equation of state were taken to be water: $\rho_{ref} = 1000$, $A = 10^5 \text{ Pa}$, $B = 3.31 \times 10^8 \text{ Pa}$, $N = 7.15$, $p_{sat} = 2 \text{ kPa}$, and $\chi_{cav} = 0.9$. The length of the domain measured one meter and was discretized with 400 cells. The diaphragm was placed at $x = 0.5 \text{ m}$. The water on the left side was at a pressure 0.1 GPa and the water on the right side at atmospheric pressure. The CFL number was set to 0.5 and RK3 was used to integrate the hyperbolic terms. The computed results are shown in Figure C.13. The exact and calculated results are very close.

C.7 Vacuum Riemann Problem with Cavitation

In this section the performance of the hyperbolic solver for a strongly cavitating liquid is examined. The settings for the equation of state and the integration routine are identical to the liquid shock tube problem. In this problem the pressure on both sides of the diaphragm was 0.1 GPa, but the liquid on the left side is initialized with a velocity of -100 m/s and the
liquid on the right side is initialized with a velocity of 100 m/s. A comparison of the exact solution to the computed solution is shown in Figure C.14, which match fairly well.

The initial condition produces a very strong rarefaction wave that propagates away from the diaphragm. The velocity is non-zero at the diaphragm and the pressure is mathematically zero due to the very high velocity difference between the left and right states. The condition where pressure and density are mathematically zero is called the so-called vacuum Riemann solution. The non-zero velocity at the center represents the spallation velocity of a cavitating mixture, which is produced by the rarefaction wave relation for a cavitating mixture being unable to match the initial velocity jump even if the pressure is zero in the starred state.
Figure C.14: Comparison of the calculated and exact solution for the vacuum Riemann using the hybrid flux evaluation scheme for several grid resolutions.

(a) Pressure

(b) Velocity

(c) Density
REFERENCES


Vita
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Ryan Houim was born on November 28, 1980 and grew up in the plains of Rugby, North Dakota. After graduating from Rugby High School, he attended North Dakota State University where he graduated with honors and received a Bachelor of Science degree in Mechanical Engineering and a minor in Mathematics in May 2004. At the Pennsylvania State University, he has worked on several projects at the High Pressure Combustion Laboratory (HPCL) including; interior ballistics of rockets and mortar systems, ablative material erosion, heat flux gauge design, and aluminum particle combustion experiments in addition to this work. He was also a Graduate Teaching Fellow from January 2011 through May 2011 and taught ME 302: Engineering Thermodynamics and Heat Transfer.