THE INFLUENCE OF DISSIPATIVE NUMERICS ON SHOCK INTERACTION MODELING FOR HYPERSONIC FLOWS

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ABSTRACT OF THE THESIS

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This paper presents a low order simulation of a hypersonic shock tunnel experiment at the Calspan-University at Buffalo Research Center (CUBRC). In this experiment, a relatively low enthalpy flow is passed over a double cone geometry at a speed near Mach 12. Empirical data is taken and a higher order simulation of the experiment is also used for comparison. The present study compares the low fidelity data (first order spatial reconstruction) against the empirical and higher fidelity data (second order reconstruction) for this flow. A large difference in separation zone length is evident between the high and low order simulations when pressure and heat transfer are plotted. This confirms the dissipative nature of low order numerical schemes. An evaluation of chemistry models is made as well, comparing the Park model with Kang & Dunn's. Little difference is observed between the low order Park results and the low order Kang & Dunn data. The Kang & Dunn model is chosen because it requires fewer computational resources.

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Dedication

To my parents, Neal and Miaoli Stoffers, who gave me a foundation upon which I could build an aerospace career.

Table of Contents

Ał	ostra	ct		ii
Ac	knov	wledge	ments	iii
De	edica	tion .		iv
Lis	st of	Tables	5	viii
Lis	st of	Figure	es	ix
1.	Intr	oducti	\mathbf{ion}	1
	1.1.	Motiva	ation	1
	1.2.	Relate	d Studies	1
	1.3.	Object	tive of Research	4
2.	Met	hodol	ogy	6
	2.1.	Govern	ning Equations	6
		2.1.1.	Inviscid Flow	6
			Conservation of Mass	6
			Conservation of Momentum	7
			Conservation of Energy	7
			Equation of State	8
		2.1.2.	Viscous Flow	8
			Conservation of Mass	8
			Conservation of Momentum	8
			Conservation of Energy	9
			Equation of State	9
		2.1.3.	Reactive Flow	9

		Conservation of Mass	10
		Conservation of Momentum	11
		Conservation of Energy	12
		Conservation of Vibrational Energy	13
		Equation of State	13
	2.2.	Flow Variables	14
	2.3.	Boundary Conditions	14
		2.3.1. Inviscid Flow	16
		2.3.2. Viscous Flow	17
		2.3.3. Reactive Flow	17
		Kang & Dunn Model	18
		Park Model	18
0	C		10
3.	Con	nputational Methods	19
	3.1.	Finite Volume Algorithm	19
		3.1.1. Discretization	19
		3.1.2. Control Volume Formulation	20
		3.1.3. Reconstruction	21
		3.1.4. Limiting	22
	3.2.	Inviscid Flux	22
	3.3.	Viscous Flux	24
		3.3.1. Differentiation	26
	3.4.	Chemical Source	27
	3.5.	Temporal Integration	27
4.	Res	$ults \dots \dots$	30
	4.1.	Flow Field	30
	4.2.	Grid Convergence	36
	4.3.	Chemistry Model	37
	4.4.	Algorithm Accuracy	38

5.	Con	clusions	42
Aŗ	open	dix A. Symbols Used	44
	A.1.	Latin Symbols Used as Variables	44
	A.2.	Greek Symbols Used as Variables	46
AĮ	open	dix B. Origin of Data	48
	B.1.	Freestream Quantities	48
	B.2.	Calculation of Mach Number	48

List of Tables

1.1.	Freestream Quantities for Select CUBRC Double Cone Experiments	3
2.1.	Prescribed Freestream Quantities	16
2.2.	Initialized Quantities	16
3.1.	Properties the Roe Matrix $\tilde{\mathbf{A}}$ Must Satisfy	23
B.1.	Source of CUBRC Experimental Data	48

List of Figures

1.1.	Double Cone Geometry	2
2.1.	Double Cone Flow Domain	15
3.1.	Changes to Computational Grid	20
4.1.	Inviscid Pressure on the Fine Grid	31
4.2.	Viscous Flow Features	32
4.3.	Contour Lines of Reversed Flow	33
4.4.	Mach Number of Reactive Flow	34
4.5.	Viscous Surface Data	35
4.6.	Reversed Flow with Surface Pressure Shape	36
4.7.	Grid Convergence	37
4.8.	Sensitivity to Grid Resolution	38
4.9.	Chemistry Model Comparison (Coarse Grid)	39
4.10.	Sensitivity to Chemistry Model (Coarse Grid)	39
4.11.	Assessment of Solution Quality	41
4.12.	Solution Quality in Regions of Interest	41

Chapter 1

Introduction

1.1 Motivation

Advancements in propulsion over the last decade have made new hypersonic vehicle designs feasible. NASA funded projects like the X-51 show promise for new government applications of the technology, and the retirement of the space shuttle has contractors analyzing hypersonic flow cases more than ever. Hypersonic flight could find its way into commercial business as well. The second phase of ESA's LAPCAT project continues to fund research for a commercial transport touted to provide cost effective, environmentally friendly flight in excess of Mach five [26]. Additionally, if Virgin Galactic's suborbital spaceflights are successful, commercial spaceflight firms may find it profitable to push higher, into the hypersonic regime.

Such advanced technologies must be proven, however, to make these exciting designs a reality. Unfortunately, research budgets are tight and using flight test for concept validation is prohibitively expensive. Improvements to the accuracy of computational fluid dynamics (CFD) must be made to allow for computational analysis of aerothermodynamics as a lower cost alternative.

1.2 Related Studies

Hypersonic flow over a double cone geometry is a frequently used test case for the validation of CFD codes. Specifically, a $25^{\circ}/55^{\circ}$ double cone has been examined by academia, in industry, and even by NATO. It is characterized by an initial cone with a half angle of 25° , as measured from the axis of symmetry. It then rises further to a half angle of 55° as seen in Figure 1.1. Here, it is depicted as a union of three simple solids. A solid



Figure 1.1: Double Cone Geometry

geometric representation was chosen because of its increasing popularity in the aerospace industry. The high repute of this representation is mainly due to cost savings; parametric solids enable engineers to make rapid design changes and even automate these changes in an optimization process [25].

Much experimental data for this configuration has been gathered at the Calspan-University at Buffalo Research Center (CUBRC) by Michael Holden. The CUBRC double cone model measures 7.625 inches from base to tip. The first cone has a 25° half angle and is 3.625 inches long. The model then flares into the second cone, of half angle 55°, which continues for 2.42552 inches in depth. The geometry flattens out to the base, which is 1.57448 inches thick. This model has been run in their first Large Energy National Shock (LENS-I) tunnel under many different flow conditions to gather data for computational studies.

While a large number of double cone experiments were conducted at CUBRC, a few runs are particularly relevant to the test studied in this paper, and are listed in Table $1.1.^1$ First, the double cone was tested under the low enthalpy *Run 28* conditions to assess the

¹Sources for these values are listed in Appendix B

impact that model misalignment or nose blunting would have on the surface data [4, 5, 21]. Another low enthalpy test, Run 35, was conducted with a higher Mach number [4]. The stagnation enthalpy was then raised to that of Run 40, and while Holden determined the flow to be steady, simulations by many CFD experts indicated unsteady flow. The total enthalpy was then raised again for the high enthalpy test, Run 42 [22]. Good agreement was once again found between computational and experimental data at this condition. Two more runs, Run 46 and Run 50, were set up based on the Run 42 test. Both runs used similar conditions, except that the total enthalpy was higher for Run 42, and the model nose was rounded for Run 50 [22]. The rounded tip was analyzed to determine the effect of strong stagnation at the tip of the geometry [22]. Lastly, the Run 80 condition was tested to learn more about the discrepancy found while simulating Run 40. The predominant change between the runs was Reynolds number, which was roughly halved for Run 80. This is the experiment that this study focuses on, but a variety of experts have run many simulations, and have compared their data to that of these tests.

	M	u_1	h_0	T	ho
Experiment		[m/s]	$\left[MJ/kg \right]$	[K]	$[10^{-3kg/m^3}]$
Run 28	9.59	2664	3.55	186	0.655
$\operatorname{Run}35$	11.30	2713	3.68	139	0.552
$\operatorname{Run}40$	11.54	3094	5.38	173	2.52
$\operatorname{Run}42$	11.46	4065	9.17	303	1.34
$\operatorname{Run}46$	11.54	3947	7.79	282	1.96
$\operatorname{Run}50$	11.60	3904	7.62	273	1.51
$\operatorname{Run}80$	11.68	3067	5.28	166	1.29

Table 1.1: Freestream Quantities for Select CUBRC Double Cone Experiments

After computations were run that greatly overpredicted the heat transfer to the model, Nompelis et al. began a simulation of the tunnel's nozzle flowfield [20]. It was discovered that the vibrational modes of the pure nitrogen flow were freezing near the nozzle throat, raising the vibrational temperature downstream. They showed the importance of modeling vibrational nonequilibrium by correcting for this and achieving a much better prediction of heat transfer [20]. In 2002, Roy et al. compared direct simulation Monte Carlo (DSMC) and Navier-Stokes methods for modeling the hypersonic double cone flow [24]. Using the same density mesh as the present study, they validated DSMC as a capable tool for simulating separated flow, as long as adequate grid refinement has been achieved in the recirculation region [24]. More recently, Gaitonde simulated a series of double cone cases, and evaluated the Park I chemistry model against Kang & Dunn's [8]. He was able to make good predictions for one laminar flow case, although the predicted surface pressure was of higher fidelity than the predicted heat transfer to the model [8]. His predictions for the other double cone case, however, suggested the flow was unsteady even though the LENS-I experiment produced a steady flow. A similar result is presented in Knight and Longo's 2010 paper for the NATO Advanced Vehicle Technology Group 136 (AVT-136) - all participants of the study predicted the flow to be unsteady [13]. Holden ran another test in the tunnel, designated *Run 80*, to determine the case's sensitivity to Reynolds number [13]. This is the flow configuration being studied in the present work. A similar study on a different flow case was conducted by Druguet et al. while validating their modified Steger-Warming scheme [6]. They found that the size of the double cone recirculation region was sensitive to the amount of dissipation introduced by the numerical scheme. The more dissipative numerical algorithms required a finer mesh to achieve accurate results.

1.3 Objective of Research

This study aims to evaluate high speed flow simulations and their sensitivity to the accuracy of the schemes used to compute them. The low enthalpy double cone experiment run by Michael Holden, designated *Run 80*, is used for comparison. A first order spatial reconstruction is used to predict the pressure at the surface and the heat transfer to the surface of the model. A similar computation, performed by Ioannis Nompelis, simulates Holden's experiment with a second order spatial reconstruction. This simulation is used as a baseline, and the structured, point-matched mesh for the current study is obtained directly from Nompelis to minimize sources of error. The grid is modified slightly (as described in Section 3.1.1) to make it compatible with the computational software package that is used. For the low order simulation, Aerosoft's General Aerodynamic Simulation Program (GASP) is used. This multi-block, cell centered, and scalable finite volume code offers multiple thermochemical models for nonequilibrium flow modeling. Two of these nonequilibrium chemical models are compared in this work. Both the Park model and the Kang & Dunn model are evaluated using low order schemes, to determine their impact on the simulated results.

Chapter 2

Methodology

2.1 Governing Equations

The equations that describe fluid motion are introduced here in differential form, without derivation.¹ Since this study analyzes flow under multiple assumptions, equations are presented to define the fluid motion in each case. They appear in order of complexity.

2.1.1 Inviscid Flow

The simplest case ignores any effects that viscosity has on the flow. The fluid medium is considered homogeneous and assumed to be a perfect gas. No turbulence effects are modeled.

Conservation of Mass

Also known as the continuity equation, the conservation of mass states that the net mass flow into any volume must equal the increase of mass in the same volume. It appears as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{2.1}$$

where ρ is the density and u_i represents the Cartesian components of the Eulerian velocity of the fluid. The index notation used (subscripts i, j, k) is vector component notation unless the same index is repeated in a term. A repeated index will be representative of a sum over that index even though no summation sign is displayed [16]. This notation is known as the Einstein summation convention.

¹Derivation of the conservation equations for a non-reacting flow can be found in [30].

Conservation of Momentum

The conservation of linear momentum states that a volume's change in momentum is due to the external forces acting on it. It can be expressed as

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \rho f_j$$

with p being the static pressure and f_j being the body force per unit mass. This formulation is most often associated with Newton's second law, and the external forces can be grouped as surface forces and body forces. Body forces are conservative forces generated by objects that are not in contact with the fluid, like gravity or electromagnetic forces. The effect of body forces, however, is not within the scope of this study. Therefore the end term is dropped, leaving

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_i} = -\frac{\partial p}{\partial x_j} \tag{2.2}$$

All other forces are considered surface forces, but pressure is the only remaining force for a frictionless flow.

Conservation of Energy

There are many different ways to express the idea that energy can neither be created nor destroyed. Different forms will be presented for each type of flow, with the clearest representation selected for each. For an inviscid flow, the energy equation is given as

$$\frac{\partial \rho \varepsilon_0}{\partial t} + \frac{\partial \rho \varepsilon_0 u_i}{\partial x_i} = -\frac{\partial p u_i}{\partial x_i} + \rho f_i u_i$$

where ε_0 is the total energy per unit mass. Total energy is the combination of the kinetic energy (per unit mass) and internal energy of a particle, so $\varepsilon_0 = \varepsilon + \frac{1}{2}u_ju_j$. Assuming the fluid is calorically perfect, the internal energy per unit mass is determined using $\varepsilon = c_v T$. Here, c_v is the fluid's specific heat at constant volume and T is the static temperature of the flow.

As with the conservation of momentum, body forces are neglected. Dropping the last term in the total energy equation leaves

$$\frac{\partial \rho \varepsilon_0}{\partial t} + \frac{\partial \rho \varepsilon_0 u_i}{\partial x_i} = -\frac{\partial p u_i}{\partial x_i}$$
(2.3)

Equation of State

One more equation is needed to close the system of equations, relating independent thermodynamic properties to each other. This is known as the equation of state, and for an inviscid compressible flow it is presented as

$$p = \rho R_s T \tag{2.4}$$

where R_s is the specific gas constant [1]. The specific gas constant can be obtained by dividing the universal gas constant by the molecular weight of the fluid.

2.1.2 Viscous Flow

The viscous flow case still considers the fluid to be homogeneous, but viscosity is introduced to the flow. In order to properly model the viscous effects, the conservation laws must be altered with additional terms. The fluid is still considered laminar.

Conservation of Mass

The addition of viscosity does not change the representation of mass conservation because the fluid is still made up of a single species in chemical equilibrium. Equation 2.1 is still used.

Conservation of Momentum

Additional surface forces act on a fluid volume when the flow is considered viscous. These forces are accounted for in the new viscous stress term on the right hand side:

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ji}}{\partial x_i}$$
(2.5)

Assuming a Newtonian fluid and using the Stokes assumption, the viscous stress can be expressed as

$$\tau_{ji} = \mu \left[\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right] - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k}$$
(2.6)

where μ is the dynamic viscosity of the fluid. Here δ_{ij} is the Kronecker delta, defined such that it equals one when i = j but is zero otherwise.

When Equation 2.6 is substituted into Equation 2.5, the conservation of momentum becomes the well known equation that bears the name of Claude-Louis Navier and George Stokes:

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_i} \left[\mu \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} \right]$$

Conservation of Energy

The conservation of energy also changes with the addition of viscosity, and may be better expressed in terms of enthalpy. This formulation is given by

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h u_i}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \tau_{ji} \frac{\partial u_i}{\partial x_j}$$
(2.7)

where h is the static enthalpy and q is the heat flux. Here the static enthalpy is defined as $h = \varepsilon + p/\rho$. The heat flux occurs by conduction, which is governed by Fourier's law:

$$q_i = -\mathcal{K} \frac{\partial T}{\partial x_i}$$

The variable \mathcal{K} represents the thermal conductivity of the fluid.

Visualizing the last term in Equation 2.7 requires the expansion of a laborious double sum. It is therefore presented for the reader in the three Cartesian directions:

$$\tau_{ji}\frac{\partial u_i}{\partial x_j} = \mu \left[2\left(\frac{\partial u_1}{\partial x_1}\right)^2 + 2\left(\frac{\partial u_2}{\partial x_2}\right)^2 + 2\left(\frac{\partial u_3}{\partial x_3}\right)^2 + \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}\right)^2 + \left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3}\right)^2 + \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)^2 \right] - \frac{2}{3}\mu \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)^2$$

Equation of State

The equation of state for the viscous, compressible flow of a perfect gas is identical to that of the inviscid case. This relation was presented in Equation 2.4.

2.1.3 Reactive Flow

The governing equations for a chemically reactive flow are composed of the three laws that govern physical motion plus a conservation equation for nonequilibrium energy [30]. The most notable change from the equations presented in the preceding sections is the inclusion of multiple species in the flow. Turbulence effects are still neglected.

Conservation of Mass

The standard continuity equation must be altered for a chemically reacting flow, to account for nonequilibrium processes. For a volumetric space, the mass rate of change of a given species is not only dependent upon the flow of mass through that space, but also the nonequilibrium production of mass within [29]. The mass of each species is conserved by

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial \rho_s u_i}{\partial x_i} = -\frac{\partial}{\partial x_i} (\rho_s u_{d_i}) + \dot{w}_s \tag{2.8}$$

where ρ_s is the density of species s. The species index s will run from the first species n to the last species m, but for this study N_2 will always be the first species, represented by n. In this equation \dot{w}_s is the rate of nonequilibrium production of the species s. The two velocity terms, u_i and u_{d_i} represent the mass-averaged mixture (bulk) velocity and the species diffusion velocity, respectively. A derivation of the diffusion velocity follows below.

The mixture density ρ can be determined by summing all species densities ρ_s , and follows the convention of this study where a value is assumed to be for the mixture unless a species index is given. The exception is the diffusion velocity term, which does not have a species index. It is implied that the quantity is that of species s since it does not exist for the mixture as a whole. If Equation 2.8 is summed for all species s, the right hand side will sum to zero and the continuity equation for a non-reacting flow is recovered [19].

Diffusion Velocity Fick's law of diffusion can be used to define the diffusion velocity for a species in the presence of concentration, pressure, or temperature gradients. Diffusion due to pressure and temperature gradients can be neglected for this flow, so only diffusion due to concentration gradients will be defined here [30]. In index notation, Fick's law relates diffusion velocity to concentration gradient with

$$\rho_s \mathbf{u_d} = -D\left(\frac{\partial \rho_s}{\partial x_1} \mathbf{\hat{x}}_1 + \frac{\partial \rho_s}{\partial x_2} \mathbf{\hat{x}}_2 + \frac{\partial \rho_s}{\partial x_3} \mathbf{\hat{x}}_3\right)$$

where D is the coefficient of mass diffusivity and $\hat{\mathbf{x}}_{1,2,3}$ are the Cartesian unit vectors. Solving for diffusion velocity, this equation can be cast in terms of the species mass fraction as

$$\mathbf{u_d} = -D\frac{\rho}{\rho_s} \left(\frac{\partial(\frac{\rho_s}{\rho})}{\partial x_1} \mathbf{\hat{x}}_1 + \frac{\partial(\frac{\rho_s}{\rho})}{\partial x_2} \mathbf{\hat{x}}_2 + \frac{\partial(\frac{\rho_s}{\rho})}{\partial x_3} \mathbf{\hat{x}}_3 \right)$$

which can be a more useful form.

The diffusion coefficient can be found through a dimensionless quantity known as the Schmidt number (Sc), which relates a fluid's viscous and mass diffusion rates [30]. If a constant Schmidt number is assumed, mixture quantities can be used to relate it to the coefficient of mass diffusivity:

$$Sc = \frac{\mu}{\rho D} \to D = \frac{\mu}{\rho Sc}$$

The coefficient can then be determined using the Schmidt number, which is a known property of the fluid.

It is important to note that the diffusion velocity does not account for the total motion of a species. The species diffusion velocity is relative to the mixture coordinate frame, which is moving at a bulk velocity u_i [29]. These velocity components can be combined simply as

$$\bar{u}_{s_j} = u_{d_j} + u_j$$

to determine the mean species velocity, \bar{u}_{s_j} . As before, combining the mean mass flux of every species with

$$\rho u_j = \sum_s \rho_s \bar{u}_{s_j}$$

should recover the mass flux of the mixture.

Conservation of Momentum

The conservation of linear momentum for a reactive fluid is, at first glance, the same as Equation 2.5. The various diffusion velocities do not appear because when considered collectively, they equal zero [19]. The viscous stress term, however, is slightly different than the definition provided by Equation 2.6. The difference lies in how the dynamic viscosity is calculated; now it must be calculated for a mixture. This computation can be performed using the semi-empirical method by Wilke [31]. This algorithm calculates the mixture dynamic viscosity by

$$\mu = \sum_{\varsigma=1}^{\varrho} \mu_{\varsigma} \left[1 + \frac{1}{\chi_{\varsigma}} \sum_{\iota=1}^{\varrho} \chi_{\iota} \phi_{\varsigma\iota} (1 - \delta_{\varsigma\iota}) \right]^{-1}$$

where the dimensionless constant $\phi_{\varsigma\iota}$ is defined by the equation

$$\phi_{\varsigma\iota} = \frac{\sqrt{2}}{4} \left[1 + \sqrt{\frac{\mu_{\varsigma}}{\mu_{\iota}}} \left(\frac{\mathcal{M}_{\iota}}{\mathcal{M}_{\varsigma}} \right)^{\frac{1}{4}} \right]^2 \left[1 + \left(\frac{\mathcal{M}_{\varsigma}}{\mathcal{M}_{\iota}} \right) \right]^{-\frac{1}{2}}$$

Conservation of Energy

The conservation of energy is again presented in a total energy formulation, but for a chemically reactive flow it is more complex:

$$\frac{\partial \epsilon_0}{\partial t} + \frac{\partial \epsilon_0 u_i}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} - \frac{\partial p u_i}{\partial x_i} + \frac{\partial \tau_{ji} u_j}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\sum_{b=1}^m \rho_b h_b u_{d_i} \right)$$

Here the heat flux q is the sum of the translational, rotational, and vibrational heat flux. Again, the diffusion velocity u_{d_i} implies a species quantity (for every b from 1...m). The enthalpy per unit mass is now given by $h_b = h_b^\circ + c_{v_b}T + \varepsilon_{v_b} + p_b/\rho_b$, where h° represents the enthalpy of formation for each species. The specific heat at constant volume for each species is defined by the contribution $\frac{3}{2}R_s$ from translation plus the contribution R_s from rotation [19]. The partial pressure p_b will be described later with the equation of state, and the vibrational energy per unit mass ε_v is explained below since it is also related to the total energy.

It is important to note that the variable ϵ_0 represents the total energy *per unit volume*, in contrast to the total energy per unit mass equation given earlier. Since this case considers multiple species, the total energy is found by adding together the internal energy components for all relevant species:

$$\epsilon_0 = \sum_{b=1}^m (\rho_b c_{v_b} T + \rho_b h_b^\circ) + \sum_{b=1}^\alpha \rho_b \varepsilon_{v_b} + \frac{1}{2} \rho u_j u_j$$

The variable α is the number of diatomic species in the system. A simple harmonic oscillator is used to model the vibrational energy of each diatomic species, with characteristic temperature θ_v . The vibrational energy per unit mass is derived from this model, and is determined by the equation

$$\varepsilon_{v_b} = \frac{R_s \theta_{v_b}}{\exp(\theta_{v_b}/T_v) - 1}$$

where T_v is the vibrational temperature.

Conservation of Vibrational Energy

Only one vibrational energy equation is needed because all vibrational modes are assumed to be in equilibrium [19]. This conservation is expressed as

$$\frac{\partial \epsilon_v}{\partial t} + \frac{\partial \epsilon_v u_i}{\partial x_i} = -\frac{\partial q_{v_i}}{\partial x_i} + \dot{s}_v - \frac{\partial}{\partial x_i} \left(\sum_{b=1}^{\alpha} \rho_b \varepsilon_{v_b} u_{d_i} \right)$$
(2.9)

with ϵ_v representing the vibrational energy per unit volume and u_{d_i} as the diffusion velocity for each species *b*. This volumetric quantity is simply the sum of $\rho_b \varepsilon_{v_b}$ for all diatomic species. The q_v term is the vibrational heat flux and \dot{s}_v is the reactive source term, which models the rate of vibrational energy production. The presence of this source term is partly due to creation of diatomic species in the system. Other contributions come from the exchange of energy with the other modes of the gas. These rates are approximated with the Landau-Teller model, which uses a single exchange rate to represent the inter-modal energy transfer [29]. The source term is comprised of the summation of these parts for each diatomic species

$$\dot{s}_v = \sum_{b=1}^{\alpha} \rho_b \frac{\varepsilon_{v_b}^* - \varepsilon_{v_b}}{\tau_b} + \sum_{b=1}^{\alpha} \dot{w}_b \varepsilon_{v_b}$$

where τ is the Landau-Teller relaxation time. The equilibrium vibrational energy $\varepsilon_{v_b}^*$ is determined in a form that is analogous to ε_{v_b} , except the equilibrium (translational) temperature is used instead of T_v .

Equation of State

The equation of state in this case must be altered to compensate for the addition of species to the system. This can be done with the additive pressure rule, which states that the static pressure of a mixture can be expressed as the sum of its component pressures [18]. Each component pressure can be determined with its own compressibility factor. By neglecting intermolecular forces, the Dalton model approximates this complex relationship, and simplifies to

$$p = T \sum_{b=1}^{m} \rho_b R_{s_b}$$

Since GASP is a cell centered finite volume code, it stores the above governing equations in a slightly different, vector format. Doing this requires storage of the dependent variables in vector form. This vector, \mathbf{Q} , appears in Equation 2.10 for perfect gas cases, where again, ε_0 is the total energy per unit mass.

$$\mathbf{Q} = [\rho_n, \dots, \rho_m, \rho u_1, \rho u_2, \rho u_3, \rho \varepsilon_0]^T$$
(2.10)

For the sake of efficiency, GASP also stores the primitive variables in vector form [10]. Equation 2.11 shows this vector, \mathbf{q} , for a perfect gas.

$$\mathbf{q} = [\rho_n, \dots, \rho_m, u_1, u_2, u_3, p]^T$$
(2.11)

These vectors will require an additional term, for vibrational nonequilibrium, when thermochemistry effects are to be modeled. The vector for dependent variables becomes

$$\mathbf{Q} = [\rho_n, \dots, \rho_m, \rho u_1, \rho u_2, \rho u_3, \rho_n e_n, \rho \varepsilon_0]^T$$

and the primitive variables will be stored as

$$\mathbf{q} = [
ho_n, \dots,
ho_m, u_1, u_2, u_3, e_n, p]^T$$

where e_n represents the nonequilibrium vibrational energy of diatomic nitrogen.

2.3 Boundary Conditions

The double cone case is solved on the 2-D axisymmetric domain in Figure 2.1, depicted in blue, with flow from left to right. The corresponding flow is subject to five of the boundary conditions available in GASP. Since it is axisymmetric about the x-axis, GASP requires that the flow lie in the x-y plane. It then creates a small wedge, with side walls rotated $\pm \pi/s_0$ from the flow plane. The boundary conditions on these walls are called **Positive Axi-symmetric Wall** and **Negative Axi-symmetric Wall**; they simply rotate the velocity vector about the x-axis to the wall cell.

A 1st Order Extrapolation boundary condition is placed on the right to allow the flow to exit the domain. For each extrapolation, the cell in the domain that is adjacent to



Figure 2.1: Double Cone Flow Domain

the boundary face is denoted $\mathbf{q}(1)$. The next two cells on the other side of the boundary face are ghost cells, respectively denoted $\mathbf{q}(0)$ and $\mathbf{q}(-1)$. They have their fundamental flow properties determined by $\mathbf{q}(1)$, which can be represented by Equation 2.12 below.

$$\mathbf{q}(-1) = \mathbf{q}(0) = \mathbf{q}(1)$$
 (2.12)

Physically, information is crossing the boundary in only one direction - from inside the domain to the ghost cells. Prescribing the downstream values in this way means this exit boundary condition is only valid if all characteristic waves are leaving the domain [10]. For this to be true, the flow traveling orthogonal to the boundary must have a Mach number greater than one since the steady-state, compressible Navier-Stokes equations are incompletely hyperbolic (mixed hyperbolic-elliptic). For a region in the flow where the Mach number is less than unity, the equations take an elliptic form. This would mean a change at one point in the region would affect all other points in the region. Information would be able to travel in all directions, contradicting the boundary condition. The Mach number of the flow near the exit boundary will be analyzed in Section 4.1 to prove the partial differential equations are hyperbolic in this region.

The supersonic inflow from the left requires a freestream boundary condition where flow properties are specified by the user. This condition is designated Fixed at Q and the values for q(-1) and q(0) are set in the Physical Models section of the GASP interface. The boundary condition is prescribed using Equation 2.13

$$\mathbf{q}(-1) = \mathbf{q}(0) = \mathbf{q}(\infty) \tag{2.13}$$

where $\mathbf{q}(\infty)$ is the vector of freestream, primitive flow quantities specified by the user.

For the current study, since the inflow is laminar and aligned with the axis of symmetry, it is completely defined by the density and two other primitive values [9]. Therefore, GASP only allows for the specification of two of these quantities along with the density. The freestream fluid is homogeneously N_2 , which dictates a density $\rho(\infty)$ of .00129 kg/m^3 . The freestream static temperature $T(\infty)$ is specified at 166 K and the velocity magnitude $|\mathbf{u}|(\infty)$ is 3067 m/s. The flow enters at zero angle of attack so the velocity vector can be simplified to merely its u_1 component. This velocity, however, is too high to initialize the flow with, so a separate set of freestream quantities must be specified for initialization [11]. The freestream Mach number in the computational domain is lowered to 0.1 to initialize the flow, but the temperature remains at 166 K. These initialization quantities are also used as the reference values for non-dimensionalizing the problem. Both sets of freestream quantities are summarized in Tables 2.1 and 2.2.

Property	Value	Property	Value
$u_1 \ [m/s]$	3067.00	$u_1 \ [m/s]$	25.82
T[K]	166.00	$T \ [K]$	166.00
$p \ [Pa]$	61.43	$p \ [Pa]$	61.43
M	11.68	M	0.10
$ ho \; \left[{kg/m^3} ight]$	0.00129	$ ho \; [^{kg}\!/m^3]$	0.00129

Table 2.1: Prescribed Freestream Quantities

 Table 2.2: Initialized Quantities

The remaining boundary condition is applied at the bottom of the domain, where the flow meets the surface of the cone. This boundary condition must change with the flow type to accommodate the inclusion of viscosity and thermochemistry models.

2.3.1 Inviscid Flow

The Tangency boundary condition is applied to the surface when viscous effects are neglected. The velocity of the last cell in the flow $[\mathbf{u}(1)]$ is projected onto the boundary $[\mathbf{u}(0)]$ using

$$u_j(0) = u_j(1) - \hat{n}_{x_j}\hat{n}_{x_i}u_i(1)$$

where each \hat{n} is a component of the surface's unit normal, positive outward. Each component is then multiplied by the magnitude of $\mathbf{u}(1)$ over the magnitude of $\mathbf{u}(0)$, which ensures the speed at the boundary matches that of the flow. The remaining primitive values are set at the boundary to that of the previous cell, in the flow.

2.3.2 Viscous Flow

After viscosity is introduced, the boundary at the wall must include a no slip condition. The condition No Slip T=Twall is selected so that the wall temperature can be specified at $T_{wall} = 300 \text{ K}$. The no slip condition sets all components of the velocity to zero at the boundary. The remaining surface quantities are set from the flow domain as follows:

$$p(0) = p(1)$$

$$R_s(0) = R_s(1)$$

$$\rho(0) = \frac{p(0)}{R_s(0)T_{wall}}$$

The variable R_s represents the specific gas constant of the fluid, in this case, homogeneous N_2 .

2.3.3 Reactive Flow

The boundary condition on the cone surface must change again when thermodynamic and chemistry effects are to be modeled. The boundary condition would need to be compatible with the selected chemistry models, and Air Catalytic T=Twall: Partial is chosen. For the homogeneous N_2 flow, this condition is the same as No Slip T=Twall except for one change. Since the dissociation of molecules is possible when thermochemistry is being modeled, the catalytic boundary condition must restrict species formation at the wall. The assumption is made that N_2 will be formed as the flow contacts the surface, and N_2 is imposed as the only species on the boundary. It may seem curious that Air Catalytic T=Twall: Full is not the chosen boundary condition, since recombination of all atoms on the wall is consistent with a fully catalytic wall assumption [12]. Unfortunately, the fully catalytic boundary condition in GASP forces a mixed N_2 and O_2 composition at the surface. Therefore, the partially catalytic condition is used so that the presence of O_2 is not required at the wall.

Two chemistry models are used for comparison purposes. One is by Kang & Dunn (K&D), the other is Park's original air model, designated Park 3 in GASP. Both models are applied with the Non-Equilibrium Vibration thermodynamics model. This model places the flow in translational and rotational equilibrium, but solves for the vibrational energy using Equation 2.9.

Kang & Dunn Model

This air model originally contains seventeen reactions between five species (N_2, O_2, NO, N, O) . This is simplified, however, by the restriction of a nitrogen only flow. The species containing oxygen are eliminated, leaving only two viable reactions:

$$N_2 + N_2 \rightleftharpoons 2N + N_2$$

 $N_2 + N \rightleftharpoons 3N$

Park Model

Like the Kang & Dunn model, this one is greatly simplified with only five possible species. The original eleven species $(N_2, O_2, NO, N_2^+, O_2^+, NO^+, N, O, N^+, O^+, e^-)$ would combine to form forty-seven reactions. Instead, only seven reactions need to be modeled:

$$N_{2} + N \rightleftharpoons 3N$$

$$N_{2} + N^{+} \rightleftharpoons N + N_{2}^{+}$$

$$2N \rightleftharpoons N_{2}^{+} + e^{-}$$

$$N + e^{-} \rightleftharpoons N^{+} + 2e^{-}$$

$$N_{2} + N_{2}^{+} \rightleftharpoons 2N + N_{2}^{+}$$

$$N_{2} + N^{+} \rightleftharpoons 2N + N^{+}$$

$$N_{2} + e^{-} \rightleftharpoons 2N + e^{-}$$

Chapter 3

Computational Methods

3.1 Finite Volume Algorithm

In order to perform the desired flow simulation, both time and the continuous domain in Figure 2.1 must be divided into a set of discrete points. A point-matched grid is used, so in three spatial dimensions, each point marks a boundary for a cell. Flow information is volume averaged over each cell and passed to adjacent cells through the cell faces. After the flow has propagated in all directions, the process is repeated for the next time interval.

3.1.1 Discretization

The flow domain is approximated by a structured grid with three coordinate directions, i, j, and k. The coordinate origin is placed at the tip of the cone, in the lower left (note: as seen in Figure 3.1, this does *not* correspond to the leftmost point in the domain). The i index runs along the surface of the cone, ending where the flow exits the domain in the top right. The j direction is normal to the cone surface, where $j(\min)$ resides on it and $j(\max)$ is at the freestream boundary. The k index begins in the x-y plane and is rotated about the x-axis, positive out of the page.

The original grid, of cell dimensions 512ix256j, was obtained from Ioannis Nompelis who had previously studied hypersonic flows over the double cone geometry [20]. This grid, however, resulted in negative volumes when GASP revolved it axisymmetrically. It can be seen in Figure 3.1b that one row of cells lies below the axis of revolution, causing the negative volumes. These cells were removed, leaving the 511x256 grid shown in Figure 3.1a that contains 131,584 nodes. This new grid was considered the fine grid for this study. GASP was used to automatically sequence the grid down to a 511x128 medium grid and a



511x64 coarse grid, having 66,048 and 33,280 points, respectively.

Figure 3.1: Changes to Computational Grid

3.1.2 Control Volume Formulation

For simplicity, the governing equations of three dimensional flow are recast in the vectorized, control volume form seen in Equation 3.1. This equation is solved using each cell in the computational domain as a control volume.

$$\frac{\partial}{\partial t} \int_{V} \mathbf{Q} \, dV + \underbrace{\oint_{A} (\mathbf{F} \cdot \hat{\mathbf{n}}) \, dA}_{\text{Flux}} = \underbrace{\int_{V} \mathbf{S} \, dV}_{\text{Chemical Source}}$$
(3.1)

Here the three vectors \mathbf{Q} , \mathbf{F} , and \mathbf{S} represent the conserved variables, fluxes, and chemical source terms. The variable V is the cell volume while A is the area of a cell face. The unit normal of each cell face is denoted $\hat{\mathbf{n}}$. If the volume-averaged vector of conserved quantities is defined as

$$\mathcal{Q} = \frac{1}{V} \int_{V} \mathbf{Q} \, dV$$

then GASP can approximate Equation 3.1 with

$$V\frac{\partial Q}{\partial t} + \sum_{A} (\mathbf{F} \cdot \hat{\mathbf{n}})A = \mathbf{S}V$$
(3.2)

on the computational grid. Since GASP performs calculations with the primitive variables, the chain rule is applied to Equation 3.2 to give

$$\underbrace{V \frac{\partial \mathcal{Q}}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial t}}_{\text{Conservative}} + \underbrace{\sum_{A} (\mathbf{F} \cdot \hat{\mathbf{n}}) A}_{\text{Flux} \quad \text{Chemical Source}} \mathbf{S} V$$

where \mathbf{q} is the vector of primitive variables defined in Section 2.2.

3.1.3 Reconstruction

In order to evaluate the flux term above, the primitive variables must be known at the faces of each cell. Since only the volume-averaged data is known, it must be used to compute a local approximation of the data at the cell faces. This calculation is performed by a process known as reconstruction [10].

In GASP, reconstruction is done using a method developed by Bram Van Leer called the Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL) [28]. For cell i, the location of the left face is denoted i - 1/2 and the right face i + 1/2. Computation of the flux terms for this cell requires the state of the right side of the left face, $\mathbf{q}(i - 1/2)_r$, and the left side of the right face, $\mathbf{q}(i + 1/2)_{\ell}$. These values are approximated using the cells on either side:

$$\mathbf{q}(i-1/2)_r = \mathbf{q}(i) - \frac{1}{4} \left([1-\kappa] [\mathbf{q}(i+1) - \mathbf{q}(i)] + [1+\kappa] [\mathbf{q}(i) - \mathbf{q}(i-1)] \right)$$
(3.3a)

$$\mathbf{q}(i+1/2)_{\ell} = \mathbf{q}(i) + \underbrace{\frac{1}{4} \left([1-\kappa] [\mathbf{q}(i) - \mathbf{q}(i-1)] + [1+\kappa] [\mathbf{q}(i+1) - \mathbf{q}(i)] \right)}_{\text{Correction Term}}$$
(3.3b)

In these equations κ represents a constant that will alter the scheme type and accuracy. The constant κ can hold values of negative one, zero, one-third, or one. When κ equals one the MUSCL scheme is centered. A value of negative one makes the scheme fully upwind, while zero and one-third are considered second and third order upwind-biased, respectively. A scheme is considered upwind-biased when for a given face, the scheme uses unbalanced data. It favors cells from the left for the left side of a face, and cells from the right for the right side of a face. The fully upwind case only uses data from the same direction as the side of the face being considered. In the computations run for this study, the reconstruction selected was merely a first order scheme. That means Equations 3.3a and 3.3b were each truncated to one term. This is the simplest reconstruction method, and will be shown to cause significant numerical dissipation (amplitude error) in the solution [14].

3.1.4 Limiting

Some higher order reconstruction schemes may have trouble resolving flowfield discontinuities like shock waves. This occurs when the reconstruction uses data from both sides of the discontinuity, giving rise to unphysical local extrema in the solution [14]. These numerical (fictitious) oscillations can be reduced by making an adjustment in the reconstruction algorithm. This process is known as limiting because it limits the reconstructed value at a face such that it stays between the adjacent cell averages. The limiting is performed on the second, correction, term in Equations 3.3a and 3.3b [10]. Therefore, since those terms are not present for this study's reconstruction, no limiter is needed.

3.2 Inviscid Flux

After the primitive values are reconstructed, the flux through each cell face can be evaluated. The flux scheme chosen is a flux difference splitting algorithm. Methods of this class provide a solution that is analogous to that of a general Riemann problem [14]. Roe developed one such method that can resolve a stationary shock exactly [10]. His scheme provides an exact solution to an approximation of the nonlinear Riemann problem. Downstream of the freestream boundary, each cell (i) uses its own state and that of the next cell to define a Riemann problem at the face between them [23]. The algorithm can be presented as

$$\mathbf{F}(i+1/2) = \frac{\mathbf{F}[\mathbf{q}(i+1/2)_r] + \mathbf{F}[\mathbf{q}(i+1/2)_\ell]}{2} - \frac{|\tilde{\mathbf{A}}|}{2} \left(\mathbf{q}(i+1/2)_{r-\ell}\right)$$
(3.4)

where the notation $()_{r-\ell}$ is shorthand for subtracting the value on the left side of the face from the value on the right side. $\tilde{\mathbf{A}}$ is a constant matrix dependent upon the local conditions. This constant matrix is created such that it satisfies the items in Table 3.1. Using a method called Roe averaging, Equation 3.4 can be recast in a simpler form:

$$\mathbf{F}(i+1/2) = \frac{\mathbf{F}[\mathbf{q}(i+1/2)_r] + \mathbf{F}[\mathbf{q}(i+1/2)_\ell]}{2} - \frac{1}{2}(\mathcal{F}_1 + \mathcal{F}_2 + \mathcal{F}_3)$$

- 1. It linearly maps the vector space of \mathbf{q} to the vector space of \mathbf{F}
- 2. As $\mathbf{q}(i+1/2)_r$ and $\mathbf{q}(i+1/2)_\ell$ both $\rightarrow \mathbf{q}(i+1/2)$, $\tilde{\mathbf{A}} \rightarrow \partial \mathbf{F}/\partial \mathbf{q}$
- 3. For any left and right states, $\tilde{\mathbf{A}} \times [\mathbf{q}(i+1/2)_{r-\ell}] = \mathbf{F}[\mathbf{q}(i+1/2)_r] \mathbf{F}[\mathbf{q}(i+1/2)_\ell]$
- 4. The eigenvectors of $\tilde{\mathbf{A}}$ are linearly independent

Table 3.1: Properties the Roe Matrix $\tilde{\mathbf{A}}$ Must Satisfy

Here \mathcal{F} is a result of substituting the Roe averaged variables into $\tilde{\mathbf{A}}$ and distributing through the second term of Equation 3.4. Remembering that a repeated Cartesian index indicates Einstein summation, the components of \mathcal{F} work out to:

$$\mathcal{F}_{1} = -\frac{p_{r-\ell}}{\overline{a}^{2}} |\overline{\lambda}_{1}| \begin{bmatrix} \overline{\rho}_{n}/\overline{\rho} \\ \vdots \\ \overline{\rho}_{m}/\overline{\rho} \\ \overline{u}_{1} \\ \overline{u}_{2} \\ \overline{u}_{3} \\ \overline{\rho}_{n}\overline{\rho}_{n}/\overline{\rho} \\ \overline{h}_{0} - \frac{\overline{a}^{2}}{\overline{\gamma}^{-1}} \end{bmatrix} + |\overline{\lambda}_{1}| \begin{bmatrix} \rho_{n_{r-\ell}} \\ \overline{u}_{1}\rho_{r-\ell} + \overline{\rho}\{u_{1_{r-\ell}} - \hat{n}_{x_{1}}(\mathbf{u}\cdot\hat{\mathbf{n}})_{r-\ell}\} \\ \overline{u}_{2}\rho_{r-\ell} + \overline{\rho}\{u_{2_{r-\ell}} - \hat{n}_{x_{2}}(\mathbf{u}\cdot\hat{\mathbf{n}})_{r-\ell}\} \\ \overline{u}_{3}\rho_{r-\ell} + \overline{\rho}\{u_{3_{r-\ell}} - \hat{n}_{x_{3}}(\mathbf{u}\cdot\hat{\mathbf{n}})_{r-\ell}\} \\ (\overline{\rho}_{n}\overline{e}_{n})_{r-\ell} \\ \sum_{b=1}^{m} \overline{\beta}_{b}\rho_{b_{r-\ell}} + (\rho_{n}e_{n})_{r-\ell} + \overline{\rho}\{\overline{u}_{i}u_{i_{r-\ell}} - \overline{\lambda}_{1}(\mathbf{u}\cdot\hat{\mathbf{n}})_{r-\ell}\} \end{bmatrix}$$

$$\mathcal{F}_{2,3} = \frac{1}{2\overline{a}^{2}} \{p_{r-\ell} \pm \overline{\rho}(\overline{a})(\mathbf{u}\cdot\hat{\mathbf{n}})_{r-\ell}\} |\overline{\lambda}_{2,3}| \begin{bmatrix} \overline{\rho}_{n}/\overline{\rho} \\ \vdots \\ \overline{\rho}_{m}/\overline{\rho} \\ \overline{u}_{1} \pm \hat{n}_{x_{1}}\overline{a} \\ \overline{u}_{2} \pm \hat{n}_{x_{2}}\overline{a} \\ \overline{u}_{3} \pm \hat{n}_{x_{3}}\overline{a} \\ \overline{\rho}_{n}\overline{e}_{n}/\overline{\rho} \\ \overline{h}_{0} \pm (\overline{\mathbf{u}\cdot\hat{\mathbf{n}}})\overline{a} \end{bmatrix}$$

A bar (⁻) denotes the use of Roe averaging and $\overline{\lambda}_{1,2,3}$ are the eigenvalues of $\mathbf{\tilde{A}}$. Each eigenvalue uses this method of averaging, with $\overline{\lambda}_1 = \overline{\mathbf{u} \cdot \hat{\mathbf{n}}}, \ \overline{\lambda}_2 = \overline{\mathbf{u} \cdot \hat{\mathbf{n}}} + \overline{a}, \ \overline{\lambda}_3 = \overline{\mathbf{u} \cdot \hat{\mathbf{n}}} - \overline{a}$.

GASP computes the Roe averages as

$$\begin{split} \overline{\rho} &= \sqrt{\rho_r \rho_\ell} & \overline{\gamma} = 1 + \frac{\overline{R}_s}{\overline{c}_v} \\ \overline{\rho}_s &= \frac{\sqrt{\rho_r}(\rho_s)_\ell + \sqrt{\rho_\ell}(\rho_s)_r}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} & \overline{R}_s = \frac{(R_s \sqrt{\rho})_r + (R_s \sqrt{\rho})_\ell}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} \\ \overline{\rho_n} \overline{e}_n &= \frac{\sqrt{\rho_r}(\rho_{n_\ell} e_{n_\ell}) + \sqrt{\rho_\ell}(\rho_{n_r} e_{n_r})}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} & \overline{e}_b^* = \frac{(e_b^* \sqrt{\rho})_r + (e_b^* \sqrt{\rho})_\ell}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} \\ \overline{u}_{1,2,3} &= \frac{(u_{1,2,3} \sqrt{\rho})_r + (u_{1,2,3} \sqrt{\rho})_\ell}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} & \overline{\beta}_b = \overline{e}_b^* - \frac{R_{sb}T}{\gamma - 1} + \frac{1}{2} \overline{u}_k \overline{u}_k \\ \overline{T} &= \frac{(T \sqrt{\rho})_r + (T \sqrt{\rho})_\ell}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} & \overline{h}_0 = \frac{(h_0 \sqrt{\rho})_r + (h_0 \sqrt{\rho})_\ell}{\sqrt{\rho_r} + \sqrt{\rho_\ell}} \\ \overline{c}_v &= \frac{1}{T_{r-\ell}} \sum_{b=1}^m \frac{\overline{\rho}_b}{\overline{\rho}} \int_{T_\ell}^{T_r} c_{v_b}(\xi) d\xi & \overline{a}^2 = (\overline{\gamma} - 1) \left[\overline{h}_0 - \frac{1}{2} \overline{u}_k \overline{u}_k + \overline{c}_v \overline{T} - \sum_{b=1}^m \frac{\overline{\rho}_b}{\overline{\rho}} \overline{e}_b^* - \frac{\overline{\rho_n} \overline{e}_n}{\overline{\rho}}\right] \end{split}$$

where again, s is the species index running from $n = N_2$ to the last species m.

3.3 Viscous Flux

When viscous effects are considered, a new vector must be added to the inviscid flux to arrive at the total flux term for the system. The components of this new viscous flux vector are calculated more simply than Roe's inviscid scheme. The vector is arranged as

$$\mathbf{F} = \begin{bmatrix} \rho_{n} \mathbf{u}_{d} \\ \vdots \\ \rho_{m} \mathbf{u}_{d} \\ \left[-\tau_{x_{1}x_{1}} - \tau_{x_{1}x_{2}} - \tau_{x_{1}x_{3}} \right] \\ \left[-\tau_{x_{2}x_{1}} - \tau_{x_{2}x_{2}} - \tau_{x_{2}x_{3}} \right] \\ \left[-\tau_{x_{3}x_{1}} - \tau_{x_{3}x_{2}} - \tau_{x_{3}x_{3}} \right] \\ \left[-\tau_{x_{3}x_{1}} - \tau_{x_{3}x_{2}} - \tau_{x_{3}x_{3}} \right] \\ \left[-\mathcal{K}_{n} \frac{\partial T_{v_{n}}}{\partial x_{1}} + \rho_{n}e_{n}u_{d_{1}} \right] \\ -\mathcal{K}_{n} \frac{\partial T_{v_{n}}}{\partial x_{2}} + \rho_{n}e_{n}u_{d_{3}} \right] \\ \begin{bmatrix} \tau_{x_{1}x_{1}}u_{1} + \tau_{x_{1}x_{2}}u_{2} + \tau_{x_{1}x_{3}}u_{3} - \mathcal{K} \frac{\partial T}{\partial x_{1}} - \mathcal{K}_{n} \frac{\partial T_{v_{n}}}{\partial x_{2}} + \sum_{b=1}^{m} \rho_{b}h_{b}u_{d_{1}} \\ \\ \tau_{x_{2}x_{1}}u_{1} + \tau_{x_{2}x_{2}}u_{2} + \tau_{x_{2}x_{3}}u_{3} - \mathcal{K} \frac{\partial T}{\partial x_{2}} - \mathcal{K}_{n} \frac{\partial T_{v_{n}}}{\partial x_{2}} + \sum_{b=1}^{m} \rho_{b}h_{b}u_{d_{2}} \\ \\ \tau_{x_{3}x_{1}}u_{1} + \tau_{x_{3}x_{2}}u_{2} + \tau_{x_{3}x_{3}}u_{3} - \mathcal{K} \frac{\partial T}{\partial x_{3}} - \mathcal{K}_{n} \frac{\partial T_{v_{n}}}{\partial x_{3}} + \sum_{b=1}^{m} \rho_{b}h_{b}u_{d_{3}} \end{bmatrix}$$

where u_d represents the diffusion velocity of that species. For each species, the diffusion velocity is calculated using a form of Fick's law

$$\mathbf{u_d} = -\frac{\rho D}{\rho_s} \begin{bmatrix} \frac{\partial(\rho_s/\rho)}{\partial x_1} \\ \frac{\partial(\rho_s/\rho)}{\partial x_2} \\ \frac{\partial(\rho_s/\rho)}{\partial x_3} \end{bmatrix}$$

where the binary diffusion coefficient D is determined using a constant Schmidt number, as described in the following paragraph. The last two vectors in the viscous flux vector are components of the conservation equations for nonequilibrium vibrational energy and total energy, respectively. Each vector component of the vibrational energy equation contains a partial derivative in a Cartesian direction, as well as a component of the species diffusion velocity in the same direction. The N_2 species-specific thermal conductivity \mathcal{K}_n is for the frozen vibrational mode, and is calculated by $\mathcal{K}_n = \mu_n c_{v_n}$. The components of the total energy equation contain similar terms.

A Schmidt number of 0.7 was used to determine the diffusion coefficient. This was done

with the relation

$$D = \frac{\mu_s}{\rho Sc}$$

where Sc is the Schmidt number and μ_s is the species viscosity. The viscosity of each species is determined with the Sutherland model, where intermolecular attraction is assumed to be weak unless molecules are in contact [10]. The species viscosity μ_s is obtained with

$$\mu_s \approx \mu_{\rm ref} \left(\frac{T}{T_{\rm ref}}\right)^{\frac{3}{2}} \frac{T_{\rm ref} + S}{T + S}$$

where μ_{ref} and T_{ref} are reference values and the effective temperature S is the Sutherland constant [30]. The mixture viscosity is then determined by Wilke's mixing rule.

3.3.1 Differentiation

The derivatives in the viscous flux vector are calculated using a finite difference scheme that Aerosoft calls *thin-layer gradients*. For all scalar variables η , this is essentially the forward Euler method

$$\frac{\partial \eta}{\partial x_i}(j+1/2) = \frac{\eta(j+1) - \eta(j)}{\Delta X} \mathbf{\hat{n}}_i$$

where ΔX is the division of a volume term by an area term. This volume is calculated by averaging the volumes of cells j and j + 1, while the face area between them is calculated using the nodes. The accuracy of a gradient calculated by this method is mainly dependent upon two grid characteristics. First, it is best for the normal at a face center to pass through the center of both adjacent cells. When this condition is nearly satisfied, the gradient approximation will be good. Relative cell size is also important, as accuracy is lost if cells in close proximity have dissimilar volumes.

At a wall boundary, a second order wall gradient is selected to approximate the derivative. It is computed with the one sided scheme

$$\frac{\partial \eta}{\partial x_i}(j) = \frac{-\eta(j+2) + 7\eta(j+1) - 6\eta(j)}{\Delta X} \hat{\mathbf{n}}_i$$

where ΔX is now the volume of the wall-adjacent cell divided by the area of the face at the boundary.

This thin layer gradient method is used to calculate the flux through each face along each parametric coordinate direction. For increased accuracy, the i - j cross derivative terms are enabled. This adds a term from the j direction calculations to the i direction flux, with the reverse being true as well. For a given face in the j - k plane, the added term incorporates the flux from the four adjacent i - k faces. A simple average of the four j direction gradients is performed; this value is then added to the original i direction flux.

3.4 Chemical Source

The vector of source terms is only present for chemically reactive flows. It contains terms for the production of species, and appears as

$$\mathbf{S} = \begin{bmatrix} \dot{w}_n \\ \vdots \\ \dot{w}_m \\ 0 \\ 0 \\ 0 \\ \dot{w}_n e_n + \rho_n \dot{e}_n \\ 0 \end{bmatrix}$$

where again, \dot{w} is the rate of nonequilibrium production of a species, and \dot{e} is defined as the rate of production of nonequilibrium energy for a species. The first set of non-zero terms represents the production of mass in the continuity equation. The other non-zero term is a part of the conservation equation for nonequilibrium vibrational energy.

3.5 Temporal Integration

The time derivative is the last remaining portion of Equation 3.1 that requires a numeric scheme. An iterative method is used to calculate the flow parameters after each discrete time step, but first the equation must be linearized. For the sake of simplicity, the vector quantities in Equation 3.1 are grouped such that \mathbf{F}' represents the flux terms, \mathbf{S}' the source terms, and $\frac{\mathbf{Q}'}{\partial t}$ the conservative terms. Linearization is performed with the implicit Euler scheme, which is first order accurate in time and unconditionally stable [27]. The implicit

Euler method changes Equation 3.1 to

$$\frac{\mathbf{Q}^{\prime(n+1)} - \mathbf{Q}^{\prime(n)}}{\Delta t} = \mathbf{S}^{\prime(n+1)} - \mathbf{F}^{\prime(n+1)}$$
(3.5)

where $()^{(n)}$ signifies the current time (when quantities are known) and $()^{(n+1)}$ represents one time step later. In this way, the time derivative of the conservative term is evaluated using the forward Euler scheme, and the flux and source terms are not known yet. These implicit right hand side terms are approximated locally as

$$(\mathbf{S}' - \mathbf{F}')^{(n+1)} = (\mathbf{S}' - \mathbf{F}')^{(n)} + \mathbf{J}^{(n)}(\mathbf{Q}'^{(n+1)} - \mathbf{Q}'^{(n)}) + \text{higher order terms}$$

where the higher order terms are dropped. The matrix \mathbf{J} is the flux Jacobian, which is a matrix of all the partial first derivatives relating $(\mathbf{S}' - \mathbf{F}')$ to \mathbf{Q}' . This local approximation is inserted into Equation 3.5, giving

$$\mathbf{Q}^{\prime(n+1)} - \mathbf{Q}^{\prime(n)} = \Delta t (\mathbf{S}^{\prime} - \mathbf{F}^{\prime})^{(n)} + \Delta t \mathbf{J}^{(n)} (\mathbf{Q}^{\prime(n+1)} - \mathbf{Q}^{\prime(n)})$$

after both sides have been multiplied by Δt . Noting the presence of $(\mathbf{Q}'^{(n+1)} - \mathbf{Q}'^{(n)})$ on both sides, it can be grouped with the similar term on the left

$$(\mathbf{I} - \Delta t \mathbf{J}^{(n)})(\mathbf{Q}^{\prime(n+1)} - \mathbf{Q}^{\prime(n)}) = \Delta t(\mathbf{S}^{\prime} - \mathbf{F}^{\prime})^{(n)}$$

after the whole term is moved to the other side. The matrix \mathbf{I} is the identity matrix. The left hand terms can now be distributed

$$\underbrace{(\mathbf{I} - \Delta t \mathbf{J}^{(n)})}_{\mathbf{A}} \underbrace{\mathbf{Q'}^{(n+1)}}_{\mathbf{x}} = \underbrace{\Delta t (\mathbf{S'} - \mathbf{F'})^{(n)} + (\mathbf{I} - \Delta t \mathbf{J}^{(n)}) \mathbf{Q'}^{(n)}}_{\mathbf{b}}$$

and the known conserved quantities can be moved to the right. Grouping the known terms on the left into a coefficient matrix (**A**), and the terms on the right into a matrix of known quantities (**b**), the above matrix equation takes the common form $\mathbf{A}\mathbf{x} = \mathbf{b}$. This equation can be solved by a direct method or through iteration [7].

Iterative schemes typically require less memory than direct methods, so iteration is used for this study [17]. In order to obtain a solution, an initial guess is chosen, and then improved upon repeatedly. The common form of $\mathbf{A}\mathbf{x} = \mathbf{b}$ is changed slightly to accommodate the improvement of \mathbf{x} , and appears as

$$\mathbf{A}_1 \mathbf{x}^{k+1} = \mathbf{A}_2 \mathbf{x}^k + \mathbf{b}$$

where $()^k$ represents the stage of iteration. The values of \mathbf{A}_1 and \mathbf{A}_2 differ depending on the chosen scheme. For a standard Gauss-Seidel formulation, the original matrix of coefficients is split into three matrices

$$\mathbf{A} = \mathbf{U} + \mathbf{D} + \mathbf{L}$$

where **U** is the upper triangular portion, **D** is the diagonal portion, and **L** is the lower triangular portion of **A**. Then $\mathbf{A}_1 = \mathbf{D} + \mathbf{L}$ and $\mathbf{A}_2 = -\mathbf{U}$. This results in

$$(\mathbf{D} + \mathbf{L})\mathbf{x}^{k+1} = \mathbf{b} - \mathbf{U}\mathbf{x}^k$$

and $(\mathbf{D} + \mathbf{L})$ can be inverted to solve for the \mathbf{x}^k to be used in the next iteration.

This solution method can be improved by performing a backward sweep through the cells after the forward sweep is performed in the standard Gauss-Seidel. This improved algorithm is called the Symmetric Gauss-Seidel method, and the new intermediate step is represented by $()^{k+\frac{1}{2}}$. The forward Gauss-Seidel is calculated as before,

$$(\mathbf{D} + \mathbf{L})\mathbf{x}^{k+\frac{1}{2}} = \mathbf{b} - \mathbf{U}\mathbf{x}^k \tag{3.6}$$

except the next iterative index is replaced by the intermediate step. Then the backward Gauss-Seidel

$$(\mathbf{D} + \mathbf{U})\mathbf{x}^{k+1} = \mathbf{b} - \mathbf{L}\mathbf{x}^{k+\frac{1}{2}}$$
(3.7)

is used to reach the next step of iteration. Combining equations 3.6 and 3.7 gives

$$\mathbf{x}^{k+1} = (\mathbf{D} + \mathbf{U})^{-1}\mathbf{L}(\mathbf{D} + \mathbf{L})^{-1}\mathbf{U}\mathbf{x}^k + [(\mathbf{D} + \mathbf{U})^{-1} - (\mathbf{D} + \mathbf{U})^{-1}\mathbf{L}(\mathbf{D} + \mathbf{L})^{-1}]\mathbf{b}$$

which simplifies to

$$\mathbf{x}^{k+1} = (\mathbf{D} + \mathbf{U})^{-1}\mathbf{L}(\mathbf{D} + \mathbf{L})^{-1}\mathbf{U}\mathbf{x}^k + (\mathbf{D} + \mathbf{U})^{-1}\mathbf{D}(\mathbf{D} + \mathbf{L})^{-1}\mathbf{b}$$

giving the Symmetric Gauss-Seidel method. This equation is solved repeatedly, improving the guess each time, until the convergence criteria is met. Then the time step is advanced by one and the process begins again.

Chapter 4

Results

Using the described numerics, this study simulates the Run 80 experiment at CUBRC. The experiment passed a flow of pure diatomic nitrogen over the $25^{\circ}/55^{\circ}$ double cone at approximately Mach 12. Ioannis Nompelis also simulated this experiment, using more accurate numerics than are presented in this paper. His finite volume code also used an implicit model, but chose the Data-Parallel Line Relaxation (DPLR) algorithm in time [22]. His inviscid flux was calculated using a hybrid Steger-Warming flux vector splitting method that does not require a limiter. Second order inviscid reconstruction was performed with an upwind MUSCL scheme and the viscous reconstruction used a second order central difference. The fine grid contained 512x256 cells and chemical reactions were modeled with Park rates. His simulation was computed using sixteen processors on a Compaq XP1000 AlphaStation cluster.

In contrast, this study uses Roe's flux difference splitting method and a first order MUSCL reconstruction for the inviscid flux. Since the inviscid reconstruction is first order, no limiter is needed. Viscous differentiation is performed using the thin-layer gradient finite difference scheme. Symmetric Gauss-Seidel iteration solves the temporal system of equations, and all runs are performed to a steady state. The fine grid for this study contains 511x256 cells. Jobs are run on a Debian Linux cluster made up of 24 AMD Dual Core Opteron processors running at 2.4 gigahertz with 24 gigabytes of RAM.

4.1 Flow Field

The double cone is an interesting geometry to study because of the interactions that occur between the laminar boundary layer and the shocks that form at high speeds. It is beneficial to begin studying this flow field in the absence of viscosity. This allows for the resolution of the far field shock structure without a boundary layer present. Figure 4.1a plots static pressure in the inviscid domain, depicting some major shock features. An oblique shock (1) forms as the flow reaches the geometry, emanating from the stagnation point at the tip of the cone. The shock continues downstream until it intersects the detached shock (2) formed by the change in the cone's half angle. At this point - known as a triple point - a reflected shock (3) forms and extends toward the cone surface. The reflected shock interacts with another shock (4) before it reaches the wall. This fourth shock turns the flow, originally processed by the first shock, so that it is nearly parallel with the second cone.

Shocks three and four are of opposing families, and their intersection results in the refraction of both shocks [1]. A magnified depiction of this region appears in Figure 4.1b. One refracted shock continues to the cone surface, finally bringing the near-wall flow to parallel. The other reaches a slip line and is reflected as an expansion wave. Another expansion occurs just before the flow leaves the domain, as the geometry of the second cone flattens out to the base.



Figure 4.1: Inviscid Pressure on the Fine Grid

The flow structure changes somewhat when viscosity is introduced to the flow, most notably near the cone surface. Figure 4.2b shows static temperature contours near the triple point. A plot of temperature reveals flow features that one of pressure cannot. A thin boundary layer is apparent along the end of the first cone, distinguished by low temperature along the cone surface. It appears even thinner on the surface of the second cone. The boundary layer cannot be visualized with pressure contours because static pressure is constant across a boundary layer. An explanation for changes in boundary layer thickness is offered toward the end of this section.

A contact discontinuity, or slip line, is also visible on the temperature chart. Like a boundary layer, the pressure on either side of the slip line must be equal by definition [1]. However, since the entropy changes across it, it is visible as a line separating the two temperature regions behind the detached shock in Figure 4.2b.



Figure 4.2: Viscous Flow Features

Additional flow features are presented in Figure 4.2a. Unlike Figure 4.1, the initial oblique shock does not intersect the bow shock from the 55° cone. Instead, an additional shock is present due to the separation of the boundary layer, as the flow encounters the resulting pocket of recirculating flow. This separation shock forms because the recirculation region changes the effective wall shape, appearing as a compression corner to the flow. The shock continues downstream until it reaches the detached shock at the triple point.

The flow that is processed by the separation shock has yet to 'feel' the presence of the second cone. As it approaches the change in geometry, it doesn't experience a sudden compression like in the inviscid case. This is once again due to the presence of the separation



Figure 4.3: Contour Lines of Reversed Flow

region, which can be visualized in Figure 4.3b. It appears as the pocket of low Mach number flow against the double cone. Referring back to Figure 4.2b, a correlation can be found between this area and the thicker boundary layer. In fact, it is the low speed that allows for the increase in boundary layer height. A theoretical analysis shows that laminar boundary layer thickness is inversely proportional to the square root of the Reynolds number, which is lower for the recirculating flow [3]. It is important to note that this zone continues outside the marked contours of reversed flow. The contours only serve to provide a relation between the separated flow and the related shock in Figure 4.3a. The smoother outer shape of this region allows for the formation of weaker compression waves, which coalesce into one oblique shock. That is why this shock appears at a non-zero distance from the wall - it is actually attached to the effective shape of the surface. The coalesced shock continues downstream and intersects the shock reflected from the triple point. The interaction between these shocks is similar to that of the inviscid case, except one refracted shock marks the reattachment point as it reaches the wall.

In all flow cases, the flow expands around the corner created by the end of the second cone and exits the domain. The speed of the flow near this boundary is of particular interest because of the boundary condition that is used. To help visualize this, Figure 4.4a presents the flow field of the entire domain in terms of Mach number. Unfortunately, this figure alone



Figure 4.4: Mach Number of Reactive Flow

does not validate the exit boundary condition. As described in Section 2.3, the component of the flow traveling orthogonal to the boundary must have a Mach number greater than one.

A simple trigonometric analysis is conducted to ensure this condition is met. The acute angle formed by the exit boundary and the base of the model is 48.31°. The assumption is made that the direction of the flow near the boundary is offset no farther than the horizontal - a rotation of 41.69° from the boundary normal. If the Mach number of the orthogonal component of the flow must be greater than unity, the Mach number of any horizontal flow must be greater than 1.339. This forms a conservative constraint on the flow near the domain exit. Figure 4.4b shows only the flow regions with a Mach number greater than 1.339. The flow at the exit boundary is shown to have an adequate Mach number, making the boundary condition a valid choice.

For the purpose of vehicle configuration design, it is more useful to analyze how these flow features affect the double cone surface. As an example, surface data is plotted in Figure 4.5 for both pressure and heat transfer. These plots allow for improved visualization of relevant data for comparison purposes. They also depict major features of the flow. The initial jump in pressure seen in Figure 4.5a is a strong adverse pressure gradient along the wall in the streamwise direction. This is the reason for separation of the boundary layer, as the fluid downstream of this point flows in the reverse direction. Therefore, this marks the separation point in the flow. The heat transfer plot in Figure 4.5b also illustrates the recirculation zone in an obvious way. Since the Mach number of the flow in this region is comparatively low, the cone surface is exposed to less heat flux. This appears on the graph as a sharp reduction in heat transfer.



Figure 4.5: Viscous Surface Data

On both charts, the separation zone is followed by a large spike in the dependent variable. This corresponds with the location of boundary layer reattachment, where the refracted shock impinges on the wall. Both values drop off shortly thereafter as they are processed by the expansion slightly downstream. Finally, before the flow exits the domain, both heat transfer and pressure drop significantly due to the expansion corner made by the end of the geometry.

A clearer comparison of surface data and flow features is made in Figure 4.6 below. The contours are of the u_1 velocity for only the reversed flow. The normalized and translated surface pressure data is plotted on top of this for qualitative purposes only. It can be seen that the first rise in surface pressure occurs near the initial point of reversed flow. The largest rise in pressure also appears near the downstream-most point of reversed flow (reattachment), as expected.



Figure 4.6: Reversed Flow with Surface Pressure Shape

4.2 Grid Convergence

A thorough study of grid convergence is necessary to ensure that the level of grid refinement used does not affect the quality of the solution. One such study was performed on this configuration by Ioannis Nompelis, for a flow case with slightly less total enthalpy [20]. His simulations were performed on four grids, of cell resolution 2048x1024, 1024x512, 512x256, and 256×128 . The computed heat transfer on the 1024×512 and 512×256 grids showed very little variance for most of the flow field, but the 512x256 grid did not resolve the separation bubble well enough. However, the data on the 2048x1024 and 1024x512 grids were nearly identical in this area, indicating grid convergence was achieved on the 1024x512 mesh. The same flow was studied by Druguet et al. and the grid resolution needed was found to be dependent on the solution method. For schemes with minimal numerical dissipation, a cell resolution of 512x256 was adequate to resolve all flow features [6]. Therefore, the 512x256mesh was chosen for this study, to examine the effect of a dissipative solution method. It was from Nompelis's study that the 512x256 grid was obtained, and altered to 511x256 for the present simulation. The medium and coarse grids were derived from this fine mesh, and a similar comparison using heat transfer is shown in Figure 4.7. The data presented is for the viscous simulation using the nonequilibrium vibration thermodynamics model and the Kang & Dunn chemistry model. The regions of interest have been magnified in Figure 4.8. The



Figure 4.7: Grid Convergence

approximate separation zone length, measured from initial drop off to peak heat transfer, varies by 33.71% between the coarse and medium grids. The percent change from medium to fine was 29.75%. This disparity makes it obvious that grid convergence has not been achieved on the 511x128 medium grid. Convergence is not determined for the resolution of 511x256 because this comparison is made in Section 4.4. Noting that the peak heat transfer only changes by 0.62% and 1.87% as the grids are refined, it is evident that separation zone length is far more sensitive to changes in grid resolution. Figure 4.8 also shows that a drop in peak magnitude is associated with a larger recirculation zone. Increased separation delays reattachment too, moving the peak heat transfer farther downstream on the cone surface. This happens because the separation zone size affects the shape and strength of the shock interactions, which in turn dictate where the refracted shock contacts the wall [6].

4.3 Chemistry Model

Two methods were used to simulate the chemical reactions taking place in this high speed flow. As described in Section 2.3.3, the Kang & Dunn model uses two reactions between two chemical species. The Park model uses seven reactions between five species. For both models, the computed heat transfer to the surface is determined using identical solution



Figure 4.8: Sensitivity to Grid Resolution

methods on the 511x64 coarse grid, and the results are plotted in Figure 4.9. Globally, the results produced by each model are nearly identical. Magnified views of the regions of interest are provided in Figure 4.10. It should be noted that the separation zone appears slightly longer as calculated by the Park model, but the location of the peaks are the same. The magnitude of the maximum heat transfer is slightly higher when the Park model is used. These slight differences, however, are achieved while incurring high computational cost. The CPU time required for the Park calculation was 8.58 times what the Kang & Dunn model needed. Consequently, the Kang & Dunn chemistry model was used for all subsequent calculations done in this study.

4.4 Algorithm Accuracy

The final results from this study are assessed in a comparison with two other datasets. One is the experimental data provided by Michael Holden, from the LENS-I tunnel at CUBRC, designated *Run 80*. The second is a simulation of Holden's experiment by Ioannis Nompelis, using the methods described at the beginning of Chapter 4. These datasets are plotted against each other in Figure 4.11. Both sets of computed data were simulated on grids of similar resolution - 512x256 for Nompelis and 511x256 for GASP.



Figure 4.9: Chemistry Model Comparison (Coarse Grid)



Figure 4.10: Sensitivity to Chemistry Model (Coarse Grid)

The difference between the computed separation zone shapes is noticeable. The separation from Nompelis matches that of the experiment much closer than the GASP results. The root cause of the disparity lies in the lower order numerics used for the GASP computations. The first order reconstruction, as Section 3.1.3 alluded, suffers from artificial dissipation that shrinks the recirculation region. This 'smearing' of the solution increases the mixing in the simulated separation zone in an unphysical way [6]. Since this makes the recirculation zone smaller, it also decreases the strength of the separation shock. This moves the refracted shock, and therefore the location of maximum heat transfer, upstream. Figures 4.12a and 4.12b provide a larger view of the heat transfer to the wall in these regions. The GASP peak in heat transfer occurs roughly 1.6cm earlier than the peak in Nompelis' data. It should be noted that the maximum experimental heat transfer isn't necessarily a good baseline for comparison since capturing the peak depends on the placement of instrumentation.

With that being said, the difference in peak heat transfer to the surface is reasonably small. The lower order scheme slightly underpredicts the magnitude of the maximum heat transfer. This is because the flow is processed by a weaker separation shock; the refracted shock must be stronger to slow the flow down more before it reaches the wall. When the low order data is compared to Nompelis' data, the percent error is about 14%. Compared to the experimental data, however, the percent error is only about 5.5%. This is a reasonable value, considering the estimated experimental uncertainty for heat transfer is 4% [15]. The magnitude and location of recovery heat transfer, downstream of reattachment, also matches well.



Figure 4.11: Assessment of Solution Quality



Figure 4.12: Solution Quality in Regions of Interest

Chapter 5

Conclusions

This study examines the impact spatial reconstruction accuracy has on numerical simulation. A first order algorithm is used to model the complex interactions between shocks and the boundary layer in laminar flow, and the results are compared to second order data. The study uses a first order MUSCL scheme to reconstruct the primitive flow variables at each cell face so that Roe's method can be used to evaluate the inviscid flux. The Symmetric Gauss-Seidel method is used to solve the temporal problem through iteration. These lower order results are presented against those of Ioannis Nompelis. His higher order schemes include a hybrid Steger-Warming method with a second order upwind MUSCL reconstruction, and an implicit solution with DPLR in time. Both sets of data are plotted against the empirical results obtained by Michael Holden at CUBRC. His experimental data is obtained from the LENS-I reflective shock tunnel. In his test, he passes a pure nitrogen flow over a $25^{\circ}/55^{\circ}$ double cone geometry, at a velocity of almost Mach 12. The data collected includes pressure at the model surface as well as heat transfer to the surface.

Two different sets of chemical equations are used to model the reactive flow with the lower order algorithm. The Park model produced slightly different results than Kang & Dunn's for both pressure and heat transfer. The Park model, however, required over eight and a half times the computational cost in order to produce these results. Since the difference between the predictions from the models was well within the experiment's estimated uncertainty for pressure (3%) and heat transfer (4%), further computations were continued with the Kang & Dunn model [15].

When comparing the pressure and heat transfer from the lower order simulation against the higher order one or experimental data, a disparity is apparent in separation region length and peak location. The dissipative nature of the lower order scheme shrinks the recirculation region substantially. This results in a premature peak and a change in shock strength, which can be visually identified by the decrease in peak magnitude. Unlike the peak location, however, the lower order peak magnitude compares reasonably to the experimental results. The location and magnitude of the recovery heat transfer also matches the higher order data well. Therefore, some flow features can be resolved reasonably by the lower order scheme, but other, more dissipation sensitive features cannot. It is important to note that the higher order simulated data overpredicts the separation region length slightly and the peak pressure and heat transfer magnitude as well, but the fidelity of the higher order data is in all cases greater than that of the lower order data. This confirms that first order spatial reconstruction, while it can be run quickly, does not produce adequate quantitative results. It should only be used to identify trends between flow cases. At least a second order reconstruction is needed to match experimental results or, in the future, predict flight conditions with confidence.

Appendix A

Symbols Used

A.1 Latin Symbols Used as Variables

Symbol	Description
a	speed of sound
A	area
Α	coefficient matrix for iteration in time
Ã	Roe constant matrix
() _b	species summation index
b	matrix of known quantities for iteration in time
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
D	coefficient of mass diffusivity
D	diagonal portion of the coefficient matrix for iteration in time
e^*	equilibrium internal energy (translational & rotational)
e	nonequilibrium vibrational energy
\dot{e}	rate of production of nonequilibrium vibrational energy
f	body force per unit mass
$\mathcal{F}_{1,2,3}$	matrices of Roe averaged values
\mathbf{F}	vector of fluxes
\mathbf{F}'	grouping of flux terms
h	static enthalpy
h_0	total or stagnation enthalpy
$()_{i,j,k}$	Einstein summation and vector indices

(continued on the next page)

Symbol (cont.)	Description (cont.)
(i, j, k)	grid location indices
i,j,k	parametric coordinate indices
Ι	identity matrix
J	flux Jacobian matrix
$()^k$	iteration index
\mathcal{K}	thermal conductivity
() _ℓ	left side of a cell face
\mathbf{L}	lower triangular portion of the coefficient matrix for iteration in time
$()_{m}$	index of the last species
M	Mach number
\mathcal{M}	molecular weight
$()^{(n)}$	time index
$()_{n}$	index of the species N_2
\hat{n}	component of the unit normal vector, relative to the surface
î	unit normal vector, relative to a cell face
p	static pressure
q	component of heat flux
q_v	component of vibrational heat flux
q	vector of primitive quantities
\mathcal{Q}	volume averaged vector of conserved quantities
Q	vector of conserved quantities
\mathbf{Q}'	grouping of conservative vector terms
$()_{r}$	right side of a cell face
R_s	specific gas constant (gas constant for a species)
$()_{s}$	species index running from ($\)_n$ to ($\)_m$
\dot{s}_v	rate of production of vibrational energy
S	Sutherland constant
Sc	Schmidt number, relating a fluid's viscous and mass diffusion rates

(continued on the next page)

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S	vector of chemical source terms
\mathbf{S}'	grouping of source vector terms
t	time
T	static temperature
T_v	vibrational temperature
u	component of the mass averaged (bulk) velocity
$u_{1,2,3}$	x, y, and z components of the velocity vector
\bar{u}	component of mean velocity
u_d	component of species diffusion velocity
u	velocity vector
$\mathbf{u}_{\mathbf{d}}$	species diffusion velocity vector
U	upper triangular portion of the coefficient matrix for iteration in time
V	volume
\dot{w}	rate of nonequilibrium production
$x_{1,2,3}$	Cartesian coordinate direction components
x,y,z	Cartesian coordinate axes
x	matrix of unknowns for iteration
$\mathbf{\hat{x}}_{1,2,3}$	unit vector in Cartesian coordinate directions
Х, Ү	Distance in Cartesian directions $x_{1,2}$

Symbol (cont.) Description (cont.)

A.2 Greek Symbols Used as Variables

Symbol	Description
α	number of diatomic species
eta	Roe scheme total energy equation constant
γ	ratio of specific heats
δ_{ij}	Kronecker delta of indices i, j
$\delta_{arsigma\iota}$	Kronecker delta of indices ς, ι

(continued on the next page)

Symbol (cont.)	Description (cont.)
ϵ_v	vibrational energy per unit volume
ϵ_0	total energy per unit volume
ε	internal energy per unit mass
ε_v^*	equilibrium vibrational energy per unit mass
ε_v	vibrational energy per unit mass
ε_0	total energy per unit mass
η	arbitrary scalar flow variable
$ heta_v$	SHO characteristic temperature of vibration
L	molecule summation index
κ	MUSCL constant
$\lambda_{1,2,3}$	eigenvalues of the Roe constant matrix
μ	dynamic viscosity
ξ	variable of integration
ρ	static density
Q	number of molecules per unit volume
ς	molecule summation index
au	component of the viscous stress
τ	Landau-Teller relaxation time
ϕ	dimensionless Wilke constant
χ	mole fraction

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Appendix B

Origin of Data

B.1 Freestream Quantities

Experiment	M	$u_1 \ [m/s]$	$h_0 \left[{MJ/kg} \right]$	T[K]	$\rho \left[10^{-3kg/m^3} \right]$
Run 28	9.59 ^a	2664^{a}	$3.55^{\rm c}$	186^{a}	0.655^{a}
$\operatorname{Run}35$	11.30^{a}	2713^{a}	$3.68^{\rm c}$	139^{a}	0.552^{a}
Run 40	11.54 ^b	$3094^{\rm f}$	5.38^{f}	$173^{\rm f}$	2.52^{f}
$\operatorname{Run}42$	11.46 ^b	4065^{f}	9.17^{f}	$303^{\rm f}$	1.34^{f}
Run 46	11.54 ^d	3947^{d}	7.79^{c}	$282^{\rm d}$	$1.96^{\rm d}$
$\operatorname{Run}50$	11.60 ^b	$3904^{\rm e}$	$7.62^{\rm c}$	$273^{\rm e}$	1.51^{e}
$\operatorname{Run}80$	11.68^{b}	3067^\dagger	5.28^{f}	166^{f}	1.29^{f}

^a From Candler et al. [4]

^b Calculated as in Section B.2

^c Approximated by $\frac{1}{2}u_1^2$ in accordance with Nompelis et al. [20]

^d From Nompelis et al. [21]

^e From Nompelis et al. [22]

^f From Knight et al [15]

[†] From Candler group data files provided by Doyle Knight

Table B.1: Source of CUBRC Experimental Data

B.2 Calculation of Mach Number

The Mach number of a flow, M, can be calculated as

$$M = \frac{|u_1|}{a} \tag{B.1}$$

where $|u_1|$ is the speed of the fluid and *a* is the speed of sound [14]. Assuming that the fluid is an ideal gas, the speed of sound can be calculated by

$$a = \sqrt{\gamma R_s T} \tag{B.2}$$

with γ as the ratio of specific heats, R_s being the specific gas constant, and T representing static temperature. The specific gas constant for nitrogen can be found by dividing the universal gas constant by the molar mass of diatomic nitrogen. The universal gas constant is taken to be 8.314 $\frac{J}{mol \cdot K}$ and the molar mass of N_2 is 28.02 $\frac{g}{mol}$ [18], [2]. The ratio of specific heats for nitrogen is approximated to be 1.4. With this information, the Mach number for each run can be calculated by inserting Equation B.2 into Equation B.1 to give

$$M = \frac{|u_1|}{\sqrt{\gamma R_s T}}$$

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