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MODELING OF NON-EQUILIBRIUM EFFECTS ON A DOUBLE WEDGE CONFIGURATION IN HYPersonic FLOWS

BY

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THESIS
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Abstract

Numerical simulations are extensively used for the modeling of hypersonic flows characterized by thermal and chemical non-equilibrium phenomena. The accurate modeling of non-equilibrium effects relies on knowledge of reaction rate constants and relaxation parameters, often extrapolated outside their range of applicability.

The objective of this thesis is the validation of the non-equilibrium models conventionally used by the scientific community. To this aim, the flow over a double wedge configuration is simulated for a nitrogen and air gas mixture at hypersonic conditions. The results are compared with experimental work performed at the University of Illinois by Austin and Swantek. The flow governing equations are discretized and solved using a parallel cell centered finite volume solver within COOLFluiD. The accuracy of the simulations is second order in space and first order in time. The convective fluxes are discretized using the AUSM+ scheme and the time is carried out using the fully implicit Backward Euler scheme.

The numerical predictions obtained show significant extent of thermal non-equilibrium between vibrational and translational energy modes, whereas chemical non-equilibrium is present only in the air case, since nitrogen molecules do not significantly dissociate. Two different observables are used for the validation: wall heat-flux, and Schlieren experimental data. In general, the numerical predictions are in good agreement with the experimental results. Only minor differences are observed in the heat flux or the shock structure configuration in the air and nitrogen cases.
To my family
Acknowledgements

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Chapter 1

Introduction

Earth’s atmosphere at sea level and ambient conditions, consists of a mixture of atoms and molecules; namely molecular nitrogen, molecular oxygen, carbon dioxide, argon and other species in minor quantities. At room temperatures and speeds significantly lower than the speed of sound, air can be modeled as a perfect gas. However, at air speeds that are much faster than the speed of sound, the perfect gas model breaks down and new physical phenomena ensue. These phenomena are now broadly outlined [23]:

- Above temperatures of 800K, the internal energy modes of the molecules and atoms present in the gas are excited and become important parameters to be modeled. Thermodynamic properties such as specific heat, internal energy, enthalpy and entropy, now need to be treated as functions of temperature.
- With a further increase in temperature, dissociation and recombination of the air molecules becomes important and thermodynamic properties need to be treated as functions of the chemical composition as well.
- Thermal – nonequilibrium begins to play a significant role. That is, the internal modes of energy are no longer in equilibrium with the translational mode of energy.
- At high enough temperatures, ionization of the gas into a plasma can occur. Along with ionization, comes the added complexity of having to account for the associated electromagnetic fields and forces.
- At temperatures above 10000K, radiation becomes a significant factor and needs to be modeled in such cases. This is primarily due to the emission and absorption of photons by the gas molecules caused by the excitation of their electrons.
- Finally, the chemically reacting gases can interact with the surface of the vehicle, affecting heat release at the wall. These situations are commonly seen in the usage of ablative heat shields.
Hypersonic flows are characterized by a freestream Mach number greater than 5. Such flows are encountered in several situations such as atmospheric re-entry, scramjet engines, high enthalpy wind tunnels and high powered lasers. The present work addresses the study of atmospheric entry applications. Most of the phenomena discussed for high temperature flows can be seen in figure (1.1)

![Flow features associated with a capsule upon re-entry](image)

**Figure 1.1: Flow features associated with a capsule upon re-entry**

In the case of hypersonic vehicles, the associated heat flux to the vehicle surface is managed with the use of heat shields and accurate prediction of these heat fluxes is essential to correctly design the required heat shielding. Conducting full scale experiments of a hypersonic vehicle (say in a very large hypersonic wind tunnel) such as a space shuttle is impossible. This is primarily because of the associated complexities in having to accelerate such a mass of air to hypersonic speeds and maintaining these speeds for the experimental observation time. Furthermore, generating a flow with a meaningful stagnation enthalpy, close to the kind of enthalpies that would be encountered in practice, is prohibitively difficult on full scale models. Instead, scaled down experimental rigs are constructed, where it is feasible to accelerate the mass of gas to the required operating conditions. These scaled down experimental results are used to validate computer solvers and to verify that the solver can capture the gas behavior with sufficient accuracy. Some common test cases used to benchmark hypersonic solvers are the cylinder case and the double wedge case.
Respectively, these cases involve a cylinder geometry and a double wedge geometry placed in a flow with a Mach number much greater than one. Experimental data on these cases is available and simulations are performed to compare against these experimental results.

The present work focuses on a double wedge case in nitrogen and air atmospheres, under the operating conditions presented in table (5.1). The purpose of this work is to validate experimental results available on the same case and contribute to the body of work on the double wedge case.

1.1 Current Work – Introduction

This thesis presents the results for simulations on a double wedge case in hypersonic flow at a Mach number of 7.14. The simulations were run on the COOLFluiD architecture, using a finite volume, cell centered solver.

The double wedge problem is a case used for testing the validity of thermochemical models and the applicability of solver code and is widely used as a benchmarking tool. The flow over a double wedge consists of complex fluid dynamic phenomena. Accurate prediction of parameters such as wall heat fluxes and pressure distributions depend on accurately capturing the fluid dynamic phenomena and using an appropriate thermochemical model.

Two time accurate cases were run for a nitrogen and air atmosphere. In general, the flow features seen in double wedge flows are shown in figure (1.2). One oblique shock attached to the tip of the wedge, one bow shock ahead of the second wedge face and the recirculation zone can be easily seen. The cases simulated show a large degree of thermal non-equilibrium and are illustrated in further sections. The geometry of the test case is detailed in table (1.1).
Figure 1.2: Double wedge geometry and flow features [1]

<table>
<thead>
<tr>
<th>Geometrical Feature</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fore Wedge Length</td>
<td>$L_f$</td>
<td>43.993 mm</td>
</tr>
<tr>
<td>Aft Wedge Length</td>
<td>$L_a$</td>
<td>25.400 mm</td>
</tr>
<tr>
<td>Forward wedge angle</td>
<td>$\alpha$</td>
<td>30.0°</td>
</tr>
<tr>
<td>Aft wedge angle</td>
<td>$\theta_w$</td>
<td>25.0°</td>
</tr>
</tbody>
</table>

Table 1.1: Geometrical Data for the Double Wedge

Experimental Data

The numerical results have been validated with experimental data for the heat transfer to the wedge surface from the work of Austin and Swantek [1]. The free stream parameters of the flow are detailed in table (5.1). The experimental work was performed in the Hypervelocity Expansion Tube (HET) at the University of Illinois, Urbana Champaign. The HET is a 9.14m long expansion tube facility, consisting of a driver, driven, and accelerator section internal diameter of 150mm. It can operate at Mach numbers of 3.5-7.5 and achieve stagnation enthalpies of 2.1-8.8 MJ/kg. This is a different “initial condition” than the initial conditions imposed in the present work where an impulsive Mach 7.14 flow is imposed throughout the flow field at the start of the simulation.

Schlieren images were captured with a Nikon zoom lens (f = 70 – 300 mm) in a Z-type schlieren system. A Xenon spark is used for illumination with a pulse width time of 20 nanoseconds. Heat flux measurements were obtained by using nineteen coaxial thermocouples with a response time of 1 microsecond. The heat
transfer values were averaged after establishing steady state. The error in heat fluxes are ±8% of the absolute value reproduced in this thesis.

1.2 Literature Review

The work by Davis and Sturtevant on double wedge geometries provides experimental and numerical data on double wedge flows [2]. The computational code in the study used a finite volume, Reynolds-averaged Navier-Stokes solver. The work used the mixing rules provided by Gupta et al [3] to calculate transport properties and the Bartlett et al [4] model for dissociation. The paper also mentions the presence of 3D effects and states that span wise measurements of flow properties showed no consistent behavior. Of interest also, are the comments on the separated shear layer and Reynolds number effects.

Numerical heat transfer results for a double cone geometry are presented in the work by Gaitonde and Canupp [5]. Along with numerical and experimental results, the paper details some flow features involved in hypersonic flows over a cone, which are similar to the flow features encountered in wedge flows. This work is a good starting point for an introduction to wedge and cone flows.

The numerical work by Badr and Doyle [6] provides computational results to for a double wedge case in both air and nitrogen environments, for the experimental work by Austin. The work provides data on the steady state establishment times and wall heat flux data for a perfect gas approximation of the flow properties. The results obtained for the Mach 7.14 case by Badr and Doyle show steady state establishment times of 1.2 to 1.8 ms depending on the grid size. The heat transfer profiles for this case differs significantly from the experimental results. Further investigation on the real gas effects for this case was recommended. Also, the impulsive start initial condition, which is not the same as the experiment was questioned as a suitable initial condition.
DSMC (Direct Simulation Monte Carlo) computations by Tumuklu, Patil and Levin [7] for double wedge flows in a nitrogen environment use the “Statistical Modeling In Low-density Environment” solver and the work provides 2D and 3D results. The paper mentions the importance of 3D effects in double wedge flows and provides some insight into how the recirculation zone is affected by 2D and 3D simulations.

Recent work by Komives, Nompelis and Candler [8] for a double wedge configuration uses US3D to obtain computational results in air and nitrogen atmospheres. They confirm that heat flux results show poor agreement with the experimental data by Austin when run until later flow times and that a good agreement is obtained only until the experimental run time. The computational results at the experimental times show a good agreement with experimental data.
Chapter 2

Physical Modeling

This section covers the governing equations, thermochemical models, transport property models and the thermodynamics used in the present work. The environments that are studied are nitrogen and air atmospheres, both of which can be described as a continuum for our operating conditions. This enables us to use the Navier-Stokes equations, complemented with models for chemical dissociation and internal energy non-equilibrium. The Navier-Stokes set of equations can be used when the gradients of the macroscopic properties have a characteristic length that is larger than the mean free path of the molecules in the flow. If the local Knudsen number is defined as:

\[ Kn = \frac{\lambda}{\rho} \left\| \frac{\partial \rho}{\partial \bar{l}} \right\| \]  

(2.1)

Where \( \bar{l} \) is the direction of the steepest density gradient, \( \rho \) is the mixture density and \( \lambda \) is the mean free path. The Knudsen number is the parameter used to determine the validity of Navier-Stokes methods and the NS equations are valid within the range of a Kn of 0.05 or lower. Higher Knudsen number flows, or rarified flows are analyzed using the Direct Simulation Monte Carlo method.

2.1 Governing Equations

This section presents the conservation equations for mass, momentum, energy and vibrational energy. The associated transport, thermochemical and thermodynamic terms are derived from concepts in statistical mechanics and are presented in later sections.

Mass Conservation

The species conservation equation gives us the capability to compute the mixture composition and is given by equation in terms of the partial densities of the components of the mixture.
\[
\frac{\partial \rho_i}{\partial t} + \nabla \cdot \left( \rho_i \bar{u} + \bar{J}_i \right) = \dot{\omega}_i
\] (2.2)

Where \( \rho_i \) is the mass density of species \( i \) and \( \bar{u} \) is the mean velocity of the mixture. \( \rho_i \bar{u} \) is the convective flux and the \( \bar{J}_i \) is the diffusive flux. \( \dot{\omega}_i \) is the chemical source term for the \( i \)th species.

Summing up the species continuity equations gives us the global mass conservation equation. Since the sum of mass production terms and the diffusive fluxes is zero, it can be obtained:

\[
\sum_{i \in S} \dot{\omega}_i = 0
\] (2.3)

\[
\sum_{i \in S} \bar{J}_i = \sum_{i \in S} \rho_i \bar{V}_i = 0
\] (2.4)

Where \( \bar{V}_i \) is the diffusion velocity. Equation (2.3) imposes the fact that there can be no net production or destruction of matter in the flow and equation (2.4) signifies the fact that the net mass does not diffuse. The global mass conservation equation as a consequence is given by:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{u}) = 0
\] (2.5)

Where \( \rho \) is the global density.

**Momentum Conservation**

The momentum conservation equation is given by:

\[
\frac{\partial \rho \bar{u}}{\partial t} + \nabla \cdot (\rho \bar{u} \bar{u}) = -\nabla p + \nabla \cdot \bar{\tau} \quad (2.6)
\]

Where \( \bar{\tau} \) is the viscous stress tensor, discussed in later sections. \( p \) is the mixture pressure and \( \rho \) is the mixture density.
Total Energy Conservation

The total energy equation, neglecting the radiative terms, is given by:

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \bar{u}) = -\nabla \cdot (\bar{f} \cdot \bar{u}) + \nabla \cdot \bar{q}$$  \hspace{1cm} (2.7)

H is the total enthalpy given by $H = E + p/\rho$ and $E$ is the total energy per unit mass; the sum of the internal energy of the mixture and the kinetic energy, given by:

$$E = e + (\bar{u} \cdot \bar{u})/2$$  \hspace{1cm} (2.8)

The mixture energy per unit mass $e$ and along with the diffusive flux and viscous stress tensor, are further explored in sections (2.3) and (2.4).

Vibrational Energy Conservation

The conservation of vibrational energy for a given species m is given by:

$$\frac{\partial \rho_m e_m^V}{\partial t} + \nabla \cdot (\rho_m \bar{u} e_m^V) = -\nabla \cdot \bar{q}_v + \Omega_m^{CV} + \Omega_m^{VT}$$  \hspace{1cm} (2.9)

Where $\rho_m$ is the density of species m and $e_m^V$ is the vibrational energy per unit mass of species m. $\bar{q}_v$ is the heat flux due to the conduction and diffusion of vibrational energy. The term $\Omega_m^{CV}$ represents the loss or gain of vibrational energy due to chemical reaction. $\Omega_m^{VT}$ represents the energy exchange with the translational energy modes. These terms are discussed in sections (2.3) and (2.4).
2.2 Thermochemistry

To account for the various effects present in hypersonic flows as previously discussed, a state of thermal and chemical non-equilibrium is assumed. Chemical non-equilibrium can be accounted for by calculating the mass production term $\dot{\omega}_i$ in equation (2.10) and solving an advection-diffusion-reaction equation for every species. This section covers the mass production term and its evaluation, the rate of reaction terms and the energy exchange terms seen in earlier sections.

**Mass Production Term**

The mass production term for any chemical reaction is given in the general form:

$$
\dot{\omega}_i = M_i \sum_{r=1}^{N_r} (v_i'^r - v_i'^r) \left\{ k_{fr} \prod_{j=1}^{Ns}(\frac{\rho_j}{M_j})^{v_j'^r} - k_{br} \prod_{j=1}^{Ns}(\frac{\rho_j}{M_j})^{v_j'^r} \right\}
$$

(2.10)

Where $\dot{\omega}_i$ is the net rate of production of species $i$ over all the reactions $r$, $v'$ and $v''$ are the stoichiometric coefficients of the reactants and the products, $k_f$ and $k_b$ are the forward and backward reaction rate constants, respectively.

**Reaction Rates and Park’s Model**

The reaction rate coefficient equation for the forward reaction rate or the Arrhenius equation is given by:

$$
k = C T_{avg}^n \exp\left(-\frac{T_d}{T_{avg}}\right)
$$

(2.11)

Where $k$ is the forward reaction rate coefficient, $C$ is the pre-exponential factor, $T_d$ is the activation energy. These values have been tabulated in table (2.1) for both of the mixtures used in the present work.
Table 2.1a: nitrogen mixture

<table>
<thead>
<tr>
<th>Reactions</th>
<th>M</th>
<th>C (cm³/(mol-s))</th>
<th>N</th>
<th>Td(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{N}_2 + M \rightarrow \text{N} + \text{N} + M )</td>
<td>( \text{N} )</td>
<td>3.00E+22</td>
<td>-1.6</td>
<td>113200</td>
</tr>
<tr>
<td></td>
<td>( \text{N}_2 )</td>
<td>7.00E+21</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2.1b: air5 mixture

Table 2.1: pre-exponential factor, activation energy and temperature exponent values used for the different reactions in the present work; for equation (2.11)

The backward reaction rates can be computed from the forward rates and the equilibrium reaction rate given by:

\[
k_f = k_b K_c^{eq} \quad (2.12)
\]

Where the equilibrium reaction rate \( K_c^{eq} \) is given by:

\[
\log \left( K_c^{eq} \right) = - \sum_{i=1}^{N_S} (v''_{ir} - v'_{ir}) \frac{g_i(T)}{RT} - \log(RT) \sum_{i=1}^{N_S} (v''_{ir} - v'_{ir}) \quad (2.13)
\]
\( g_i \) is the Gibbs free energy per unit mole of species \( i \) and is calculated using the statistical mechanical methods described in [9].

To account for the thermal non-equilibrium, Park’s two temperature model is used. Park’s model reserves one temperature \( T \) for the rotational and translational temperatures and another temperature for the vibrational modes, \( T_v \). These two temperatures are implemented in the chemistry by assuming that the chemical reaction rates are functions of the geometric mean between \( T \) and \( T_v \), as shown in equation (2.14).

\[
T = T^s T_v^{s-1}
\]  
(2.14)

Where \( s \) ranges from 0.5 – 0.7 [10]. The influence of this model on the chemical reaction rates is accomplished by a non-equilibrium factor, \( Z(T,T_i) \), which relates the equilibrium reaction rates to the corresponding non-equilibrium reaction rates as shown:

\[
k_f^r = Z(T, T_i) k_f^{r,eq}
\]

(2.15)

Where \( T_i \) represents the temperature in consideration while evaluating the chemistry; for example, it is taken to be the vibrational temperature when evaluating the effect of vibrational energy on dissociation.

Parks two temperature model yields \( Z \) to be:

\[
Z(T, T_v) = (T_{Avg} T^{-1})^n \exp \left( -\frac{\theta_d}{T_{Avg}} + \frac{\theta_d}{T} \right)
\]

(2.16)

Where \( T_{Avg} \) is the averaged temperature and \( \theta_d \) is the characteristic dissociation temperature of the molecule.

**Vibrational Translational Exchange** \( \hat{\Omega}_m^{VT} \)

The vibrational-translational energy exchange term is given by a Landau-Teller formula [11]:

\[
\hat{\Omega}_m^{VT} = \rho_m \frac{e_m^v(T) - e_m^v(T_{vm})}{\tau_m^{VT}(T)}, m \in \nu
\]

(2.17)

This equation is valid for the harmonic oscillator model and depends on the assumptions that:

- The transitions occur among neighboring states only
• The rate constants for these transitions are proportional to the quantum number

• The energy levels are populated according to the Maxwell-Boltzmann distribution

\[ \tau_m^{VT}(T) \] is the average relaxation time and is given by:

\[
\tau_m^{VT}(T) = \frac{\sum_{j \in H} \rho_j \rho_j}{\sum_{j \in H} \sum_{M_j^{VT}} \rho_j}
\]  

(2.18)

Where \( \tau_{mj}^{VT} \) is based on the formula by Millikan-White with Park’s correction [10]

**Vibration-Chemistry-Vibrational Exchange \( \Omega_m^{CV} \)**

The production and consumption of molecules due to the chemical reactions present in the flow affect the average vibrational energy of the gas and this is accounted for by the term \( \dot{\Omega}_m^{CV} \), which is [11]:

\[
\dot{\Omega}_m^{CV} = G_{app_{rm}} \dot{\omega}_m^f + G_{va_{rm}} \dot{\omega}_m^b
\]  

(2.19)

\( G_{app_{rm}} \) represents the average vibrational energy lost due to chemical reactions and \( G_{va_{rm}} \) represents the average vibrational energy gained due to chemical reactions. \( \dot{\omega}_m^f \) and \( \dot{\omega}_m^b \) are the destruction and production terms of molecule \( m \).

To account for the vibrational energy losses due to dissociation, Park’s model, assuming preferential dissociation and recombination of molecules in the vibrational state is used; and is given by equation (2.21) [12]. The preferential dissociation model is based on the assumption that dissociation occurs only from the upper vibrationally excited states. This imposes the consequence that molecules in lower states must climb to the higher vibrationally excited states before dissociating.

\[
G_{app_{rm}} \text{ or } G_{va_{rm}} = \hat{c}_1 \tilde{D}_s
\]  

(2.20)

This equation is an empirical relation where the average vibrational energy lost or gained due to chemical reactions is taken to be a fraction of the dissociation energy or the molecule \( \tilde{D}_s \). The values for \( \tilde{D}_s \) are tabulated in table (2.2) and work by Sharma, Huo and Park gives the value of \( \hat{c}_1 \) to be 0.3 [13]
<table>
<thead>
<tr>
<th>Species</th>
<th>$D_x$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N\textsubscript{2}</td>
<td>9.759</td>
</tr>
<tr>
<td>O\textsubscript{2}</td>
<td>5.115</td>
</tr>
<tr>
<td>NO</td>
<td>6.496</td>
</tr>
<tr>
<td>N</td>
<td>-</td>
</tr>
<tr>
<td>O</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 2.2: Molecular dissociation energies for the different species used in the present work

2.3 Thermodynamics

This section presents the modeling of the thermodynamic properties of the gas; which are derived from the concepts of statistical mechanics. The molecules and atoms of a gas can be said to possess energy that can be characterized into the following modes:

- Translational energy associated with the motion of the center of mass of atoms and molecules through space
- Rotational energy modes associated with the rotational motion of molecules
- Vibrational energy modes associated with the vibration of atoms with respect to each other within a molecule
- Internal energy modes associated with the excitation of electrons within an atom with respect to the nucleus

It should be noted that the rotational and vibrational modes are coupled to each other through a rigid – rotator and harmonic – oscillator model. The thermodynamic properties, namely energy, enthalpy and entropy are derived from statistical mechanics, using partition functions. The separability of the rotational, vibrational and electronic modes of energy gives us unique partition functions for each and are presented in equations (2.22) and (2.23). The derivation of the partition functions can be found in [14]. The derivation of the thermodynamic properties can be found in cited texts that the reader can refer to. Since the test cases...
presented in this thesis have little to no ionization observed, the electronic contributions are assumed to be negligible and are not included in the simulations.

**Rotational Partition Function**

\[
Q_{R_i} = \frac{T_R}{\sigma \theta_{R_i}} + \frac{1}{3\sigma} + \frac{\theta_{R_i}}{15\sigma T_R}
\] (2.21)

**Vibrational Partition Function**

\[
Q_{V_i} = \frac{1}{1 - \exp\left(-\frac{\theta_{V_i}}{T_V}\right)}
\] (2.22)

Where \(\theta_{R_i}\) is the rotational characteristic temperature, \(\theta_{V_i}\) is the vibrational characteristic temperature and \(\sigma\) is the symmetry number and it is equal to either 1 or 2 depending on whether the molecule is homonuclear (consisting the same atoms like \(\text{N}_2\) and \(\text{O}_2\)) or heteronuclear (consisting different atoms, like \(\text{NO}\))

**Equation of State**

The equation of state that is used is given by equation (2.24) where \(p_i\) and \(\rho_i\) are the partial pressure and the partial density, of the \(i^{th}\) species, respectively. \(R_i\) is the specific gas constant for the \(i^{th}\) species and is the universal gas constant divided by the species molar mass.

\[
p_i = \rho_i R_i T
\] (2.23)

The mixture pressure and mixture density is related to the species pressures and densities by the Dalton’s law of partial pressures:

\[
p = \sum_{i=1}^{N_x} p_i = \sum_{i=1}^{N_x} \rho_i R_i T
\] (2.24)
Translational energy, enthalpy and entropy

The translational energy for atoms and molecules per unit mass is given by equation (2.26) and is arrived at by assuming that the quantum states are populated according to a Boltzmann distribution. The translational enthalpy and entropy are given by equations (2.27) and (2.28) [15]:

\[ e_{Ti} = \frac{3}{2} R_i T \]  
(2.25)
\[ h_{Ti} = e_{Ti} + R_i T \]  
(2.26)
\[ s_{Ti} = \frac{h_{Ti}}{T} + R_i \ln \left[ \frac{2\pi m_i \hbar^2}{k_i^2} \right] + \frac{5}{2} R_i \ln(T) - R_i \ln(p) \]  
(2.27)

Where \( R_i \) is the species gas constant and \( m_i \) is the mass of the \( i^{th} \) species.

Rotational energy, enthalpy and entropy

The rotational energy and enthalpy per unit mass for a diatomic molecule behaving as a rigid-rotator, harmonic-oscillator is given by [14]:

\[ e_{Ri} = h_{Ri} = R_i T_R \]  
(2.28)

The rotational entropy is given by the equation:

\[ s_{Ri} = \frac{h_{Ri}}{T_R} + R_i \ln \left[ \frac{T_R}{\sigma_i} \left( \frac{T_R}{\theta_{Ri}} + \frac{1}{3} \right) \right] \]  
(2.29)

Vibrational energy, enthalpy and entropy

The vibrational energy and enthalpy for a molecule of a certain species \( s \) is given by equation (2.30) [15]:

\[ e_{Vi} = h_{Vi} = \frac{\theta_{Vi}}{e^{\theta_{Vi}/T_V} - 1} R_i \]  
(2.30)

Vibrational entropy is given by:

\[ s_{Vi} = \frac{h_{Vi}}{T_V} - R_i \ln \left[ 1 - \exp \left( \frac{\theta_{Vi}}{T_V} \right) \right] \]  
(2.31)
\( \theta_{Vi} \) is the characteristic vibrational temperature of species \( i \).

**Mixture energy, enthalpy and entropy**

The mixture energy per unit mass \( e \) from equation (2.33) is a summation of the mass fraction times the species energy \( e_i \) over all the species and is given by:

\[
e = \sum_{i \in S} \gamma_i e_i
\]  

(2.32)

For atoms, ignoring electronic contributions, \( e_i \) is the sum of the translational and formation energy contributions, written as functions of temperature and is given by:

\[
e_i = e_{Ti}(T) + e_i^F
\]  

(2.33)

For molecules, \( e_i \) can be written of the sum of the translational, rotational, vibrational and formation energies, written as functions of temperatures:

\[
e_i = e_{Ti}(T) + e_{Ri}(T_R) + e_{Vi}(T_V) + e_i^F
\]  

(2.34)

Where \( e_i^F \) is the energy of formation, computed from the heat of formation at 0K

The mixture enthalpy per unit mass is given by the equation (2.36) and is a summation of the mass fraction of species \( i \) times the species enthalpy:

\[
h = \sum_{i=1}^{N_S} \gamma_i h_i
\]  

(2.35)

The species enthalpy \( h_i \) for atoms and molecules is given by:

\[
h_i = e_i + R_i T
\]  

(2.36)

The mixture entropy per unit mass is given by:

\[
s = \sum_{i=1}^{N_S} \gamma_i s_i + k_B \sum_{i=1}^{N_S} \frac{n_j}{X_j}
\]  

(2.37)

Where the species entropy for atoms is the same as the translational entropy for species \( i \):
The species entropy for molecules is the sum of the translational, vibrational and rotational components:

\[ s_i = s_{Ti}(T) \]

Finally, translational and rotational specific heat ratios are given by the equation (2.41):

\[ c_{v,s}^t = \frac{3 \nu}{2M_s} \quad \text{and} \quad c_{v,s}^r = \frac{d \nu}{2M_s} \]

Where \( d \) is a constant equal to 0 for monoatomic molecules, 2 for diatomic and inline polyatomic molecules and 3 for non-inline polyatomic molecules.
2.4 Transport Properties

In the case of non-equilibrium, a molecular transport of mass, momentum and energy exists due to the presence of the gradients of thermodynamic properties such as composition, velocity and temperature. The diffusion fluxes, stress tensor and heat flux need to be estimated and are done in the MUTATION library implemented in COOLFluiD [16]. The transport fluxes are computed based on a Chapman-Enskog perturbative solution to the Boltzmann equation and are described presently.

Diffusion Fluxes

Diffusion fluxes are computed based on a Stephan-Maxwell equation and the expression for the diffusion flux can be written as [11]:

$$\frac{M}{\rho} \sum_{i \in \mathbb{H}} \left( x_{si} \vec{I}_i - \frac{x_i \vec{J}_s}{M_s D_{si}} \right) = \vec{d}_i$$

(2.41)

Where $\vec{d}_i$ is the vector of the driving forces and $D_{si}$ is the binary diffusion coefficient.

Viscous Stress Tensor

The viscous stress tensor $\overline{\tau}$ is given by [11]:

$$\overline{\tau} = \mu (\nabla \vec{u} + \nabla \vec{u}^T) \left( \kappa - \frac{2}{3} \mu \right) (\nabla \cdot \vec{u}) \hat{I}$$

(2.42)

Where $\mu$ is the shear viscosity and $\kappa$ is the contribution from bulk viscosity.

Heat Fluxes and Thermal Conductivities

$\vec{q}$ in equation (2.7) is the heat flux and is a sum of the conductive heat flux (the heat flux contributions from $T$, $T_R$ and $T_v$) and the diffusive heat flux and is presented in equation (2.43) The first three terms on the right hand side of equation (2.43) contribute to the conductive heat flux and the third term is the diffusive heat flux.
\[ \tilde{q} = -\lambda^T \nabla T_t - \lambda^V \nabla V_v - \lambda^R \nabla R_r + \sum_{i \in S} h_i \tilde{j}_t \]  

(2.43)

Where \( h_i \) is the enthalpy of the \( i \)th species and \( \lambda^T, \lambda^R \) and \( \lambda^V \) are the translational, rotational and vibrational thermal conductivities respectively. \( \lambda^R \) and \( \lambda^V \) are arrived at by means of the Eucken correction [17] and are given by:

\[ \lambda^R = \sum_{i \in H} \frac{p_i c_{pi}^R}{\sum_{j \in H} x_j D_{ij}} \]  

(2.44)

\[ \lambda^V = \sum_{i \in H} \frac{p_i c_{pi}^V}{\sum_{j \in H} x_j D_{ij}} \]  

(2.45)

c_{pi}^R and \( c_{pi}^V \) are the rotational and vibrational species specific heats per unit mass. The translational thermal conductivity and the shear viscosity are computed by solving the transport system as discussed in Ref. [18]
Chapter 3

Numerical Modeling

3.1 Finite Volume Method

COOLFluiD uses a Cell-Centered Finite Volume method where a computational domain is discretized into several smaller components called “cells”. The fluid properties at each cell is taken to be constant throughout the cell and located at the cell centroid while a change in the properties occurs across a cell boundary, from cell to cell.

The finite volume discretization is applied to the systems of governing equations is written in integral form as [19]:

\[
\frac{d}{dt} \int U d\Omega + \int \nabla \cdot F^c d\Omega = \int \nabla \cdot F^d d\Omega + \int S d\Omega \quad (3.1)
\]

Applying Gauss’s theorem to convert the volume integrals in equation (3.1) to contour integrals over the boundary of each cell gives us:

\[
\frac{d}{dt} \int U d\Omega + \oint F^c \cdot n d\Omega = \oint F^d \cdot n d\Omega + \int S d\Omega \quad (3.2)
\]

Where \( \Omega \) represents the volume of each cell. It can be noted that each term in equation (3.2) can be discretized separately and the spatial discretization is of the second order.

Convective fluxes are discretized using the Advection Upstream Splitting Method+ or AUSM+ scheme where the flux \( F \) from equation (3.2) is split into convective and pressure components. The AUSM+ scheme has certain advantages for the better resolution of flow discontinuities and fewer shock oscillations. The flux splitting is done according to equation (3.3):

\[
F = F^c + F^p = m_{1/2} \psi_{L/R} + p_{1/2} \quad (3.3)
\]

Where \( \dot{m} \), the scalar mass flux, \( \psi \), the vector quantity and \( F^p \), the pressure flux, can be expressed as:
\[ \dot{m} = M_{1/2} a_{1/2} \begin{cases} \rho_l & \text{if } M_{1/2} > 1 \\ \rho_R & \text{otherwise} \end{cases} \] (3.4)

\[ M_{1/2} = M^+(M_L) + M^-(M_R) \] (3.5)

\[ \psi = \begin{pmatrix} y_s \\ u \\ H \\ y_m E_m^v \end{pmatrix} \] (3.6)

\[ p_{1/2} = P^+(M_L)p_L n + P^-(M_R)p_R n \] (3.7)

Where \( n \) is the normal to the cell face and \( M_{1/2} \) is the interface Mach number.

The interface speed of sound \( a_{1/2} \) can be expressed with the following equations:

\[ a_{1/2} = \min(\bar{a}_L, \bar{a}_R) \] (3.8)

\[ \bar{a} = \frac{a^* \tilde{a}}{\max(a^*, |q_n|)} \] (3.9)

Where the critical speed of sound \( a^* \) is given by:

\[ a^* = \sqrt{\frac{2\tilde{\gamma}(\tilde{\gamma} - 1)}{2\tilde{\gamma} + \tilde{\gamma}(\tilde{\gamma} - 1)H}} \] (3.10)

Where \( \tilde{\gamma} \) is the frozen specific heat ratio, given by:

\[ \tilde{\gamma} = \frac{\sum S y_s \frac{\partial h_s}{\partial T}}{\sum S y_s \frac{\partial e_s}{\partial T}} \] (3.11)

And the equivalent specific heat ratio is:

\[ \tilde{\gamma} = 1 + p/\rho e \] (3.12)

Details on the split Mach number \( M^\pm \), the split pressure functions \( P^\pm \) and information on the AUSM+ method can be found on the work by Liou [20]
Venkatakrishnan Limiter

A phenomenon observed at a fluid discontinuity such as a shock is an oscillation of the fluid properties before and after the shock. One solution to solving this phenomenon was described by Barth and Jespersen [21] by introducing a limit $\phi_i$ to the gradients of the fluid properties. The limit is given by:

$$
\phi_{ij} = \begin{cases} 
\min \left(1, \frac{\max(\bar{u} - \bar{u}_i)}{u_{ij} - \bar{u}_i} \right), & \text{for } u_{ij} > \bar{u}_i \\
\min \left(1, \frac{\min(\bar{u} - \bar{u}_i)}{u_{ij} - \bar{u}_i} \right), & \text{for } u_{ij} < \bar{u}_i \\
1, & \text{for } u_{ij} = \bar{u}_i
\end{cases}
$$

(3.13)

$$
\phi_i = \min(\phi_{ij})
$$

(3.14)

The problem with the Barth-Jespersen method is the inherent non-differentiability of the function $\phi_{ij}$, leading to the non-differentiability of second order fluxes. This was fixed by Venkatakrishnan [22] by replacing the $\min(1,y)$ function with:

$$
\phi(r) = \frac{r^2 + 2r}{r^2 + r + 2}
$$

(3.15)
3.2 Time Discretization

The discretization in time is performed by a Backward Euler scheme which is fully implicit and of the first order. The scheme is given by:

$$\bar{R}(P^{n+1}) = \frac{U(P^{n+1}) - U(P^n)}{\Delta t} + R^{FV}(P^{n+1})$$  \hspace{1cm} (3.16)

Where $\bar{R}(P)$ is a pseudo-steady residual and $U = U(P)$ is an explicit relation for the conservative variables $U$. A one step Newton method gives us the system:

$$\left[ \frac{\partial \bar{R}}{\partial P}(P^n) \right] \Delta P^n = -\bar{R}(P^n)$$  \hspace{1cm} (3.17)

Where the Jacobian $\frac{\partial \bar{R}}{\partial P}$ is computed numerically. Equation (3.17) is solved using the Generalized Minimal RESidual algorithm with an Additive Schwartz preconditioner. The solution is updated into the natural variable vector $P$. 


Chapter 4

Computational Domain and Boundary Conditions

The grid built and used in the present work is shown in figure (4.1). Figure (4.1 b) shows the grid at the wedge elbow. The grid is structured and is 35000 elements in size. The grid parameters are presented in table (4.1). The grid design procedure was based on the following criteria:

- Obtaining a cell width at the wall that is small enough to be able to capture the wall heat flux gradients and capture the fluid dynamic phenomena at the wall
- An effort was made to design appropriate cell thicknesses at critical points in the flow – the cell thickness at the nose is smaller than at other sections such as the outlet wall
- The inlet line geometry is crucial to obtaining an appropriate cell alignments at important points in the flow, such as the shock locations and the recirculation zone locations
- The final grid points and inlet geometry were decided after iterating for a stable solution with several grid geometries and grid bias values

<table>
<thead>
<tr>
<th>Grid Size</th>
<th>35000 Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Grid Points</strong></td>
<td></td>
</tr>
<tr>
<td>x direction (unbiased)</td>
<td>175</td>
</tr>
<tr>
<td></td>
<td>1 (no bias)</td>
</tr>
<tr>
<td>y direction (biased)</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>1.035 bias at nose / 1.03 bias at outlet</td>
</tr>
<tr>
<td><strong>Wall cell thickness (m)</strong></td>
<td></td>
</tr>
<tr>
<td>Nose</td>
<td>0.2e-6</td>
</tr>
<tr>
<td>Elbow</td>
<td>1.61245e-6</td>
</tr>
<tr>
<td>Double Wedge End</td>
<td>1.835779e-6</td>
</tr>
<tr>
<td>Outlet</td>
<td>9.8e-6</td>
</tr>
</tbody>
</table>

Table 4.1: Grid Parameters
Figure 4.1: Grid resolution. (b) shows the grid zoomed in at the elbow of the wedge

Figure 4.2 shows the complete grid and the boundary conditions imposed at different edges. The flow is from the left to the right. The purple edge denotes the inlet, blue denotes the outlet, green the wedge wall and red denotes the edge of symmetry. The two cases for air and nitrogen worked on in this thesis both have a freestream velocity of 3812 m/s. This is imposed at the inlet, along with fixed species densities and free stream temperatures. At the outlet, we impose a zero gradient (with respect to the surface normal) boundary condition for the species densities, velocities and temperatures. The wedge surface is a no-slip, isothermal boundary condition, with fixed wall velocities (equal to zero) and temperatures. Finally, at the symmetry wall, we impose a zero gradient condition for the species densities and temperatures.

Figure 4.2: Boundary Conditions
Chapter 5

Results - Nitrogen Case

The following sections present the numerical results obtained for the Nitrogen case, taking into account a two species model for N atoms and N$_2$ molecules. The simulation was run with a time step of 1e-10 seconds until the oblique shock stabilized and which was increased to 1e-9 seconds for until 300ms was reached.

<table>
<thead>
<tr>
<th>Free stream parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach number</td>
<td>7.14</td>
</tr>
<tr>
<td>Static temperature, K</td>
<td>710</td>
</tr>
<tr>
<td>Static pressure, kPa</td>
<td>0.78</td>
</tr>
<tr>
<td>Velocity, m/s</td>
<td>3812</td>
</tr>
<tr>
<td>Mixture Density, kg/m$^3$</td>
<td>0.0038</td>
</tr>
<tr>
<td>Stagnation enthalpy, MJ/kg</td>
<td>8.0</td>
</tr>
</tbody>
</table>

Table 5.1: Free Stream Parameters

The free stream parameters for both the nitrogen case and the air5 case are presented in table (5.1). While the freestream mixture density for both cases is the same, the partial densities of each species was calculated using the mixture density and mass fractions of the species at the operating conditions.

5.1 Temperature Contours

The translational and vibrational temperature contours for this case are shown in figure (5.1). The temperatures shown range from a minimum of 298 K (fixed at the wall) to a maximum of close to 7000K. A large degree of thermal non equilibrium is present as seen. The vibrational temperatures reach a maximum close to 6000K. These two sets of figures are extracted from a range of times, starting from 0.0417ms till 0.3007ms. From the results, it was noted that the bow shock began to move downstream starting at 0.0417ms and the time evolution of the contours indicate that the bow shock begins to show some stabilization at around 0.130ms and shows little change between 0.1607ms to 0.3007ms. The vibrational temperatures however, evolve until around 0.190ms and are stable up to 0.242ms.
Translational and Vibrational Temperature contours at 0.041708 ms

Translational and Vibrational Temperature contours at 0.071708 ms

Translational and Vibrational Temperature contours at 0.100708 ms

Figure 5.1 (cont.): Translational and Vibrational Temperature contours at different times for the nitrogen atmosphere
Figure 5.1 (cont.): Translational and Vibrational Temperature contours at different times for the nitrogen atmosphere
Figure 5.1 (cont.): Translational and Vibrational Temperature contours at different times for the nitrogen atmosphere
Translational and Vibrational Temperature contours at 0.300708 ms

Figure 5.1: Translational and Vibrational Temperature contours at different times for the nitrogen atmosphere

It is expected that the steady state time for the nitrogen case, as observed from the contours, lies between 0.190ms to 0.242ms.

5.2 Shock Surface Extraction

Further data on the shock surface has been extracted and is shown in figure (5.3). The method employed to extract the shock surfaces is as follows: first, a density gradient magnitude plot is calculated and parsed into the required magnitude (figure 5.2). An image of this plot is then used to extract edges using the Roberts edge detection algorithm implemented in MATLAB. The coordinates for the origin of the shock surface plots was established by implementing the edge detection algorithm on a completely flooded contour plot of the density gradient, giving us the coordinates of the wedge geometry in the form of binary image coordinates, which were then scaled. Due to the different stages of post processing of the shock data, no smoothing functions have been applied on the plots to minimize error and the kinks seen in the plots do not reflect actual shock geometry – rather are the consequence of some minimal noise generated during image processing due to the nature of the bow shock, in particular, it’s thickness.
Figure 5.2: Gradients of density magnitude showing internal shocks, the oblique shock and the bow shock taken at 0.242 ms

It can be noted that the oblique shock does not change its angle to the wedge during the time period in consideration and remains steady. The bow shock reaches a steady state and stops moving upstream at around 0.130 ms. This further confirms the decision that a steady state is reached after 0.130 ms.

Figure 5.3: Extracted shock surfaces at different flow times
5.3 Recirculation Zone Data Extraction

The recirculation zone can be observed in figure (5.4). One major vortex can be noted followed by one smaller vortex at a position slightly upstream. Data for the extraction of the location of the recirculation zone at different times was done in the following manner: flow velocity values at a constant distance of 5E-6 m (this value is chosen for the sake of accuracy and physical meaning) from the wedge surface, parallel to the surface were extracted and plotted. The points at which the velocities change sign denote the start and end of recirculation zones. A sample velocity plot is shown in fig. and data extracted from these plots is shown in figure (5.5)

![Figure 5.4: Contour plot of temperature, with velocity vectors, illustrating the recirculation zone](image)

![Figure 5.5: Plot of y-velocity at a constant distance of 5E-6 m from the wedge wall](image)
Figure 5.6: Recirculation zone positions at different times. The solid line shows the position of the smaller vortex and the dotted line shows the position of the larger vortex.

It can be seen that the recirculation zone size and position shows little change between ~0.2 ms and ~0.242 ms – the experimental data by Austin suggests a steady state time of ~0.242 ms too. While this is a relatively small region in time to conclude that the steady state is established here, it needs to be noted that that other flow features such as the shock structure and the heat flux shows little change during these times.

5.4 Heat Transfer

Heat transferred to the wedge wall has been plotted as a function of x and can be seen in figure (5.7). It can be seen that the fluctuations in heat transfer are minimal between 0.1907ms and 0.242 ms and are similar to the heat fluxes from earlier times such as 0.0417 to 0.0717ms. The heat transfer plots have been compared with Austin and Swantek [1] and show a good degree of agreement with the experimental results.
5.5 Heat Transfer – Recirculation Zone Dependence

The figure (5.9) illustrates the close dependence between heat transfer and the start and end of the recirculation zones – and in general, the fluid dynamic phenomena. We can note that a drop in heat flux consistently occurs at the start of the recirculation zone. The inner, smaller vortex too plays a role as the heat flux drops again at the start of the inner vortex. The heat flux peaks at the location of the triple point,
and consistently, this peak is brought about after the end of the outer, larger recirculation zone. The data, recorded at different times, consistently shows the same behavior at all times.

Figure 5.9: Heat flux and recirculation zone plot overlay for times from 0.1907 to 0.242 ms
5.6 Dissociation

Contour plots of the mole fraction of N and N\(_2\) at 0.242 ms are shown in figure (5.10). As can be seen, the mole fractions of N\(_2\) remain close to 1 throughout the flow and very little (almost none) dissociation of the freestream N\(_2\) is seen. The contours are calculated from the species partial density data throughout the flow field.

![Figure 5.10: Atomic nitrogen and molecular nitrogen contours at 0.242 ms](image)

The same situation persists throughout the set of times investigated and dissociation is not present for the Nitrogen case. A perfect gas approximation of the flow is still not suitable – while minimal chemical dissociation is seen, the large degree of thermal non-equilibrium seen in the temperature contours still needs to be accounted for.
Chapter 6

Results – Air5 Case

The following sections present the numerical results obtained for the Air5 case, taking into account a five species model for N atoms, N\(_2\) molecules, O atoms, O\(_2\) molecules and NO molecules. The simulation was run with a time step of 1e-9 until the oblique shock stabilized and was increased to 1e-8 for until 330ms was reached. The increase in the time step from the Nitrogen case was done in the interest of time and computational power.

6.1 Temperature Contours

The translational and vibrational temperature contours for this case are shown in figure (6.1). The temperatures shown range from a minimum of 298 K (fixed at the wall) to a maximum of close to 7000K. As with the nitrogen case, a large degree of thermal non-equilibrium is observed. The vibrational temperatures reach a maximum of ~7000K. The contours have been extracted from a range of times, starting from 0.054ms till 0.334ms. Like in the nitrogen case, it can be noted that the bow shock began to move downstream starting at 0.054ms and the time evolution of the contours indicate that the bow shock begins to show some stabilization at around 0.174ms and shows little change between 0.214ms to 0.254ms.

![Translational and Vibrational Temperature contours at 0.054 ms](image)

Figure 6.1 (cont.): Translational and Vibrational Temperature contours at different times for the air5 case
Figure 6.1 (cont.): Translational and Vibrational Temperature contours at different times for the air5 case
Translational and Vibrational Temperature contours at 0.214 ms

Translational and Vibrational Temperature contours at 0.242 ms

Translational and Vibrational Temperature contours at 0.254 ms

Figure 6.1 (cont.): Translational and Vibrational Temperature contours at different times for the air5 case
Figure 6.1: Translational and Vibrational Temperature contours at different times for the air5 case
6.2 Shock Surface Extraction

The shock surfaces for the Air5 case have been extracted in the same way as the nitrogen case and is presented in figure (6.12). Again, the oblique shock does not change its angle to the wedge during the time period in consideration and remains steady. The bow shock reaches a steady state and stops moving upstream at around 0.174ms. It is considered that the steady state period ranges from 0.214ms onward. The schlieren for the Air5 case has been presented in figure (6.11).

Figure 6.2: Gradients of density magnitude showing internal shocks, the oblique shock and the bow shock taken at 0.242ms

Figure 6.3: Extracted shock surfaces at different flow times
From the contours of density gradients, several internal shock structures can be observed. Also to be noted is the triple point. These contours, when observed over time, show the internal shocks moving and gradually stabilizing.

### 6.3 Recirculation Zone Data Extraction

The recirculation zone plots, shown in figure (6.13) for the air5 case show fewer smaller vortices with one vortex appearing only at 0.334ms. However, the location of the recirculation region is fairly constant between 0.174ms and 0.254ms. Again, the steady state time for this case can be said to occur in this region and will be further examined in the heat flux plots. The method for extracting the locations of the recirculation region is the same as the nitrogen case. The velocity plots are shown in figure (6.14).

![Contour plot of temperature, with velocity vectors, illustrating the recirculation zone](image1)

**Figure 6.4:** Contour plot of temperature, with velocity vectors, illustrating the recirculation zone

![Plot of y-velocity at a constant distance of 5E-6 m from the wedge wall](image2)

**Figure 6.5:** Plot of y-velocity at a constant distance of 5E-6 m from the wedge wall
Figure 6.6: Recirculation zone positions at different times. The solid line shows the position of the smaller vortex and the dotted line shows the position of the larger vortex.

It can be noted in the air5 case that the inner minor vortex in the recirculation zone is not present at earlier times and the first instance of this can be seen at 0.334 ms. While the size and position of the recirculation zone remains constant from around 0.174 ms to 0.254 ms, simulations beyond 0.334 ms can be done to evaluate the presence of another steady state region in time.

6.4 Heat Transfer

The heat flux plots for the air5 case have been shown in figure (6.16) with the comparisons to the experimental data. We see some instability in the evolution of heat flux with time. However, at three distinct times from 0.214 ms to 0.254 ms, the plots are identical with very little variation and the plots shows good agreement with the experimental data. The effect of the recirculation zone on these three times is further explored in the next section. It can be noted that the size and position of the zone during these three times remain almost unchanging.
Figure 6.7: Heat flux profiles for all the times in consideration

Figure 6.8: Heat flux profiles from 0.214 ms to 0.254 ms
6.5  Heat Transfer – Recirculation Zone Dependence

The dependence of heat flux on the location of the recirculation zone in the air5 case can be seen in figure (6.18). The results are consistent in time and across for both atmospheres too. As previously observed, the triple point always occurs downstream of the recirculation region. A drop in heat flux is seen at the beginning of the region and peaks in the heat flux seem to consistently occur downstream of a vortex.

Figure 6.9: Heat flux and recirculation zone, plot overlay for times from 0.214 to 0.254 ms
6.6 Dissociation

Contour plots of the mole fractions of N, N₂, O, O₂ and NO have been presented in figure (6.19). As can be seen, a substantial amount of dissociation does occur. Most of the dissociation occurs in the bow shock region, as is to be expected. These results confirm the need to model real gas effects, for air and nitrogen. The chemistry observed in the air⁵ case cannot be ignored and plays a vital role in the accurate prediction of heat fluxes. While the contours of mole fractions presented are at 0.242 ms, dissociative effects are observed at different flow times too.

Figure 6.10 (cont.): Contours of mole fraction of different species, for Air⁵, at 0.242 ms
Figure 6.10: Contours of mole fraction of different species, for Air5, at 0.242 ms
Chapter 7

Conclusions and Future Work

The present work has analyzed hypersonic flows over a double wedge configuration for the operating conditions based on experiments by Austin and Swantek [1]. The case worked on was for the M7.8 conditions for both nitrogen and air atmospheres. Previous work by Badr and Doyle for the same test case note that further work should have been done with real gas effects taken into consideration and this thesis accomplishes that. From the results, we note some major conclusions:

- Consistently, thermal non-equilibrium is observed for different flow times, for both the air and nitrogen cases as is evidenced by the temperature contour plots
- For the nitrogen case, it can be noted that the degree of dissociation is quite small, while for the air case, a large degree of dissociation is observed, especially around the bow shock region of the flow
- The heat flux measurements show some encouraging agreement with experimental data with respect to previous work
- Comparable to the experimental data on steady state establishment times, the present work has produced similar steady state times
- A definite correlation between the heat flux distribution and the location of the recirculation zone has been observed; this correlation is consistent with the observations for the smaller vortex at the wedge elbow, too. One possible explanation for this is that, as observed in the velocity vector plots, at the start of the recirculation zone, the flow tends to flow away from the wall, thus transferring some of the heat flux back into the bulk flow. At the point where the recirculation zone ends, the velocity vectors are seen to be flowing back towards the wall, thus essentially, transferring some of the heat flux back to the wall
- The density gradient contours bring out the presence of weak shocks and the triple point within the flow
• The triple shock triple point consistently occurs after the end of the recirculation zone, prompting the question: How are these two phenomena linked?

Future Work

It can be noted that the geometry of the recirculation zone need not be symmetric in the case of a 3D simulation of the same case. Since we have observed a strong correlation between the heat flux and the recirculation zone, a 3D simulation of the case is the way forward. The current grid used is quite coarse by hypersonic standards and a better design with finer grids is necessary. A comprehensive understanding of the effect of the intermediary, weak shocks, with the heat flux is necessary. While no dissociation is observed for the nitrogen case, real gas effects, at the least for to account for the thermal non-equilibrium is essential. The simulations in this work required an approximate time of two months for the nitrogen case and one month for the air case. It can be noted that the nitrogen case was run with a time step of 1e-9 for the majority of the simulation, an increase in time step can be employed in future work, however, preliminary results with increased time steps seem to discourage this. In any case, the simulation could not handle larger time steps until the oblique shock was completely developed and this is something to note in future simulations for this case.
References


