Numerical Simulation of Chemically Reactive Hypersonic Flows

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Preface

The present thesis is the result of my work as a research scholar at the Shock Wave Laboratory of the Aachen University, Germany. Part of this work was funded by the German Research Foundation (DFG) under the Graduate study programme "Transport processes in hypersonic flow".

I am greatly indebted to Prof. Dr.-Ing. Herbert Olivier, the Institute director and my supervisor, for providing me the exciting opportunity to work on this research project, and for his competent guidance and motivation throughout the project. His diverse interest and experience in the field of hypersonic flows, played a major role in the completion of this research project. He had been very supportive to me throughout my stay at the institute. It has been a great experience to work under his supervision.

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I am especially grateful to Priv.-Doz. Dr. Siegfried Müller for the valuable help and consistent guidance on real gas modelling and grid adaptation. He has been very supportive on many occasions during this research. I would like to express my special thanks to Dr.-Ing. Frank D. Bramkamp for his consistent guidance related to the flow solver part of QUADFLOW, and Dipl.-Math. Philipp Lamby for providing the grids needed for the computations. These three people are the founder developers of the QUADFLOW and it was an enriching experience while working with them.

My special thanks goes to my colleague Dipl.-Phys. Florian Zus, who joined the institute, at the later stage of my thesis. We had so much fruitful discussions on real gas modelling, which helped me a lot in interpreting the computational results. I was fortunate to have such a colleague.

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I wish to express my thanks to all my colleagues of the Shock Wave Laboratory, for their support and the great enjoyable work environment they created in the institute. It has been a great pleasure to work with all of them.

Last, but not least, I would like to thank my wife Punam for her trust, support and encouragement throughout this research work.
Abstract

To study the atmospheric reentry phase of a space vehicle, it is necessary to understand correctly the thermochemical nonequilibrium processes coupled with the aerodynamic phenomena of this critical phase. In a typical hypersonic flow about a blunt body, the strength of the bow shock is such that the region between the body surface and shock is the site of intensive thermochemical processes. The different internal energy modes of the molecules are far from their equilibrium state. The energy exchanges between these different modes occur according to the individual relaxation time associated to each processes. Detailed physico-chemical models for air in chemical and thermal nonequilibrium are needed for a realistic prediction of hypersonic flow fields. One of the key issues in the design of a hypersonic vehicle is the evaluation of aerodynamic heating. Especially, shock-shock interference heating phenomena is an important and critical problem in the development of air-breathing hypersonic vehicles. Of special interest is the Edney type IV interaction, because it is known to generate the highest local loads in pressure and heat transfer. A number of numerical studies on shock-shock interference problems have been conducted. Most of these studies, however, assume a perfect gas model. For high-enthalpy hypersonic shock-shock interactions, however, real gas effects become important. Real gas effects can have a noticeable impact on flow features, such as shock stand-off distance in a blunt body flow and surface heating rates. Because of their importance, real gas effects have recently been the focus of several studies. An improved understanding of the influences of real gas effects on the shock interaction phenomenon reduces a significant element of risk in the design of hypersonic vehicles.

In the framework of the present work, the adaptive CFD code QUADFLOW has been extended for a five components air model. Different thermochemical models were implemented. The uncertainties associated with the physico-chemical modelling and their influence on the flow fields are discussed with the help of computational results. Further, an attempt has been made to improve the understanding of influence of the real gas effects on the type IV shock-shock interactions by the present computational study. In this regard, a series of numerical simulations of the experiments conducted at GALCIT T5 hypervelocity shock tunnel on shock-shock interactions were carried out. The computed results are discussed in comparison with the experimental results and computational results of DLR FLOWer-Code, which is a non-adaptive RANS-solver.
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List of symbols

- $\alpha$: Speed of sound [m/s]
- $C_p$: Pressure coefficient [-]
- $c$: Mole concentration [mol m$^{-3}$]
- $c_p$: Specific heat capacity at constant pressure [J/kgK]
- $c_v$: Specific heat capacity at constant volume [J/kgK]
- $D$: Diffusion coefficient [m$^2$/s]
- $D_n$: Damköhler number [-]
- $E$: Total specific energy [J/kg]
- $E_{for}$: Activation energy for reaction $r$ [J/kg]
- $e$: Specific internal energy [J/kg]
- $F_{visc}, G_{visc}$: Inviscid flux vectors in x and y directions, respectively
- $F_{visc}, G_{visc}$: Viscous flux vectors in x and y directions, respectively
- $H$: Total specific enthalpy [J/kg]
- $h_\alpha$: Specific enthalpy of species $\alpha$ [J/kg]
- $Kn$: Knudsen number [-]
- $K_{eq,r}$: Equilibrium constant for the $r^{th}$ reaction
- $k$: Thermal conductivity [W/mK]
- $k_{for}$: Forward reaction rate coefficient in $S,I$ units
- $k_{back}$: Backward reaction rate coefficient in $S,I$ units
- $Le$: Lewis number [-]
- $L_{max}$: Maximum number of vibrational states [-]
- $M$: Mach number [-]
- $M_\alpha$: Molecular mass of species $\alpha$ [kg/mol]
- $N_A$: Avogadro's number [-]
- $N_m(L)$: Number of particles of species $m$ at energy level $L$ [-]
- $N_r$: Total number of reactions [-]
- $N_s$: Total number of species [-]
- $n$: Unit normal vector
- $n_m$: Number densities of species $m$ [1/m$^3$]
- $n_{mx}, n_{my}$: Components of $\mathbf{n}$ in x and y directions, respectively
- $P_{n\rightarrow n'}$: Probability in the vibration-vibration coupling
- $P$: Pressure [N/m$^2$]
- $Q$: Partition function [-]
- $q$: Heat flux [J/m$^2$s]
List of symbols

\( \alpha \): Mass diffusion flux of species \( \alpha \) [kg/m\(^2\)s]

\( Re \): Reynold number [–]

\( Ru \): Universal gas constant [J/kgK]

\( S \): Thermochemical source term vector

\( St \): Stanton number [–]

\( T \): Translational-rotational temperature [K]

\( T_{Fr} \): Reaction temperature of forward reaction \( r \) [K]

\( T_{br} \): Reaction temperature of backward reaction \( r \) [K]

\( T_{vih} \): Vibrational temperature of species \( m \) [K]

\( t \): Time [s]

\( U \): Solution vector

\( U \): Probability temperature [K]

\( u_x, v \): Speed in x and y directions, respectively [m/s]

\( X \): Mass fraction [–]

\( Y \): Mole fraction [–]

\( z_{num} \): Number of \( m \rightarrow \eta \) collisions per unit time [1/s]

\( \rho \): Density [kg/m\(^3\)]

\( \gamma \): Ratio of specific heats [–]

\( \theta \): Characteristic temperature [K]

\( \omega \): Chemical source term [kg/m\(^3\)s]

\( \Omega \): Energy source term [J/m\(^3\)s]

\( \phi \): Limiter function

\( \Delta \): Shock stand-off distance [m]

\( \beta \): Shock angle [°]

\( \delta \): Boundary layer thickness [m]

\( \tau \): Relaxation time [s]

\( \sigma_{num} \): Collision cross-section of species \( m \) and \( \eta \) [m\(^2\)]

\( \mu \): Viscosity coefficient [kg/m\(s\)]

\( \mu_{num} \): Reduced mass of species \( m \) and \( \eta \) [kg/m\(\mu\)]

Subscripts

\( \alpha \): Chemical species

\( m, \eta \): Diatomic species

\( \infty \): Free stream condition

\( b \): Backward rate quantity

\( f \): Forward rate quantity
Superscripts

\( i \)  
Energy mode \( i \)

\( el \)  
Electronic

\( r\alpha \)  
Rotational

\( tr \)  
Translational

\( v\beta \)  
Vibrational

\( 0 \)  
Zero–point

Abbreviations

\( MW \)  
Millikan and White

\( VD \)  
Vibration–Dissociation

\( VT \)  
Vibration–Translation

\( VV \)  
Vibration–Vibration
Chapter 1

Introduction

1.1 Relevant physics of hypersonic flows

Defining the hypersonic flow regime is highly subjective and therefore open to discussion. In general, however, the hypersonic flow is best defined as that regime where certain physical phenomena become progressively more important as the Mach number is increased to higher values [2].

One of these phenomena is the presence of strong shock waves close to the surface of the body in case of an external flow around a body. As a result of the high free stream Mach number, the strong shock waves will result in high temperature and density jumps over the shock wave. The relatively small part of the flow field between the bow shock and the surface in hypersonic flow is called the shock layer. For increasing Mach numbers, the shock angle decreases, making the shock layer smaller. At the same time, the thickness of the boundary layers on hypersonic vehicles can be large relative to the thickness of the shock layer. This can be seen by considering that the laminar boundary layer thickness δ, on a flat plate grows like δ \sim M_{\infty}^2 / \sqrt{Re_{\infty}}, where \( M_{\infty} \) is the free stream Mach number and \( Re_{\infty} \) is the local Reynolds number [2]. Clearly for large \( M_{\infty} \), the boundary layer can occupy a significant portion of the flow field and in some cases, may merge with the bow shock itself. Therefore in hypersonic flows, viscous and inviscid effects interact strongly. This interaction is known as hypersonic viscous interaction. In this case, the classical concept of boundary layer fails and only a fully viscous approach should be used to model the hypersonic flow properly. The viscous interaction influences the stability of the boundary layer and the location of the shock wave. This can have a major affect on the lift, drag, and stability of a hypersonic vehicle.

Increasing the free stream Mach number from a supersonic value, the temperature behind the bow shock wave, in case of an external flow, will at certain Mach number become so high that the internal energy modes of the molecules are excited. At even high Mach numbers, the temperature can become high enough for dissociation of the diatomic gas molecules to occur. Increasing the Mach number even further can lead to ionization of some of the species. The gas may then emit or absorb radiation. In expanding regions of the flow field, the gas cools. This leads to the recombination of the constituents and relaxation of the internal energy levels. The thermochemical excitation of vibration,
dissociation, ionization and radiation are commonly referred to as high-temperature effects. These effects cause the flow properties to deviate from the perfect gas values.

Other typical features important in hypersonic flow fields are rarefaction phenomena in case the density is very low. A typical rarefaction effect is the occurrence of velocity and temperature slip at the wall of a body. The well known no-slip boundary condition is not valid anymore in this case. At low temperatures (< 800 K), a mixture of gases, such as air for example, can be modeled as a mixture of calorically perfect gases having constant specific heats, since only the translational and rotational modes of internal energy are fully excited. When the temperature of the air is increased above 800 K, vibrational excitation of the molecules may occur, and this causes the specific heats to become a function of the temperature; the gas is said to be thermally perfect. As the temperature is further increased, chemical reactions can occur and air becomes a chemically reacting mixture of thermally perfect gases. For an equilibrium chemically reacting gas, $c_p$ and $c_v$ are functions of both temperature and pressure, and hence $\gamma = f(T, p)$. For air at 1 atm pressure, $O_2$ dissociation ($O_2 \rightarrow 2O$) begins at about 2000 K, and the molecular oxygen is totally dissociated at about 4000 K. At this temperature $N_2$ dissociation ($N_2 \rightarrow 2N$) begins, and is essentially totally dissociated at about 9000 K. Above a temperature of 9000 K, ions are formed ($N \rightarrow N^+e^-$, $O \rightarrow O^+e^-$), and the gas becomes a partially ionized plasma.

The high temperature effects described above are initiated and proceed through collisions of the molecules. To reach a full excitation of e.g. the vibrational energy mode, a molecule needs to collide a number of times with other molecules. The same is true for a chemically reacting medium to reach its equilibrium composition at a given pressure and temperature. In general, these processes have characteristic time scales for reaching equilibrium. If the characteristic time needed for the thermodynamic state and chemical composition to approach equilibrium is small compared to the characteristic time of the flow, the flow is then said to be in thermochemical equilibrium. In hypersonic flow fields, the flow velocity can be very high and the density very low. The characteristic time needed for the equilibrium thermodynamic state and equilibrium chemical composition can lag those at the local pressure and temperature significantly. The flow is then said to be in chemical and thermal nonequilibrium. The situation, where only the thermal excitation is in equilibrium can also occur since the number of collisions needed for reaching equilibrium thermodynamic state is smaller than for the chemical composition to approach its equilibrium value at the local pressure and temperature. Another possibility may occur when the characteristic time needed for the thermodynamic state and chemical composition to be reached is so large that the state and composition of the gas hardly change in the flow field. Then the flow is said to be frozen.

All the phenomena described above occur at one stage during the ascent of a space vehicle towards its orbit and during descent from this orbit to the ground. The phase of the descent where the space vehicle enters the part of the upper atmosphere with a significant density is called "reentry". Usually for a space vehicle this is the part of the flight where the typical hypersonic features are important. For a space vehicle, the relevant gas dynamic problems become more challenging, since the vehicle flight trajectories traverse a wide range of Mach, Knudsen and Reynolds number. Thus the vehicle
experiences flow regimes going from subsonic to hypersonic, continuum to free molecular, and laminar to turbulent. Furthermore, the high temperature chemical phenomena introduce several widely varying Damköhler numbers. In a hypersonic flight, the full range of molecular physical phenomena encompassing: rarefaction, ionization, radiation, relaxation and equilibrium (thermal and compositional), in general, manifest themselves in macroscopically significant forms occurring over wide Ma-Kn-Re-Da ranges.

Some practical consequences of the high temperature phenomena in hypersonic (so called real gas effects) are significant changes in shock stand-off distances, peaks in thermal loads, skin friction drag, forces and moments on the vehicles [2], [91]. It is important to note that not only heat transfer and skin friction but even a pressure dependent aerodynamic quantity such as the pitching moment, can be affected by high temperature chemistry, as was observed during the Apollo missions and in shuttle flights wherein flap control deviated from the design predictions. This “pitching moment anomaly” has now been identified as mainly due to the thermochemical nonequilibrium effects inadequately simulated in wind tunnels and design codes of the 1960s [2], [91]. Thus an improved understanding of various thermochemical processes is required, in order to accurately predict the flow characteristics.

1.2 Shock-shock interaction

An important issue for the design and development of aerospace vehicles is the effect of various types of flow phenomena on aerodynamic performance and aeroheating characteristics. Of particular concern are shock-shock interactions, which can cause significant local increase in surface pressure and heating. Heating levels up to 30 times those to the undisturbed stagnation flow can be generated on the leading edge surface adjacent to the region of shock-shock interaction. Shock wave interference heating is a critical problem in the structural design of the thermal protection system and the load-carrying structure of high-speed vehicles. Some of the practical examples, where the phenomenon is observed are vehicles with a delta planform where the bow shock intersects the swept leading edge of the wing, flow paths of supersonic propulsion systems and the interaction of bow shock from the main body of a missile impinging on a side-strapped booster or fuel tank. Vehicles such as these operate in regimes that produce significant departures from thermochemical equilibrium in the flow about vehicle surfaces. Improved understanding of the influence of real gas effects on the shock interaction phenomenon reduces a significant element of risk in the design of hypersonic vehicles. A detailed flow field structure is required to predict the magnitude of the aerodynamic heating rate in such a flow field. The most complete description of the shock impingement phenomenon is due to Edney [25], who observed and categorized six distinct shock-wave interference patterns known as types I-VI, all of which can occur when an oblique shock intersects the bow shock of a leading edge. The most serious interaction pattern of interest is the so-called type IV interaction that involves a supersonic jet structure impinging nearly normal to the surface. The type IV shock-shock interaction occurs when an oblique shock wave impinges in the vicinity of the geometrical stagnation point. A number of numerical studies on shock/shock interference problem have been conducted. Most of
these studies, however, assume a perfect gas model [63], [100], [119]. For high-enthalpy hypersonic shock/shock interactions, however, real gas effects become important. The influences of the real gas effects on this design-limiting phenomenon are hitherto poorly understood. Real gas effects can have a noticeable impact on flow features, such as surface heating rates. Because of their importance, real gas effects have recently been the focus of several studies [29], [40], [88], [105].

1.3 Objective of the present work

The objective of the present work is two fold: first to enhance the understanding of the influence of thermochemical modellings on the relaxation processes in the hypersonic flow field and then in particular, to improve the understanding of the real gas effects on the the shock/shock interactions by computational means. In this study, the adaptive CFD code QUADFLOW, being developed at RWTH Aachen was used for the computations. References [12], [13], [14] describe the detailed features of the QUADFLOW code. In its basic form, the flow solver assumes a thermally and calorically perfect gas model. In the framework of the present study, the QUADFLOW code has been extended to take into account the real gas effects. Different thermochemical models have been integrated in the code. A number of typical test cases were computed and validated with the available experimental and theoretical results. The influence of different thermochemical models on the relaxation processes have been investigated using one-dimensional study of relaxation processes behind a stationary normal shock and a two-dimensional flow field over a circular cylinder. The various aspects of different thermochemical models are discussed in detail. Finally the investigation of real gas effects on the shock-shock interactions were carried out. The present study mainly concentrates on type IV interference pattern, since the heating rates for remaining regimes are less intense and therefore not design limiting. In this regard, the flow solver QUADFLOW was applied for the numerical simulations of the experiments carried out by Sanderson [88] on shock-shock interactions. In the experiment, three different test conditions were used, which are given in Table 6.1. The first test condition, case A, represents a low enthalpy control condition where the only real gas effects are a partial excitation of the vibrational modes in the stagnation regions of the flow. Case C represents a high enthalpy condition that was chosen to highlight the influence of nonequilibrium thermochemistry on the problem. Case B is an intermediate enthalpy condition that was designed to aid interpretation of the differences in the flow mechanisms for cases A and C. Sanderson [88] concluded as a result of the experimental studies that the real gas effects cause an increase in the scale of interaction region which results in a reduction in the peak heating enhancement, which are in contrary to the variable $\gamma$ model of Edney [25]. In the context of the present work, the computations were performed for all the three test cases of Sanderson and the computed flow characteristics and the surface Stanton number distributions were discussed in comparison with the experimental results. Further, some of the major difficulties that can be encountered in computational simulation of such flows are highlighted.
Chapter 2

Physical modelling

In this chapter, the governing equations for a multi-species gas that is thermally excited and chemically reacting, are described. The formulations of Gnooffo et al. [33] are followed in describing the equations. These equations are based on the Navier-Stokes equations which are statements of global continuity: total mass conservation, total momentum conservation and the total energy conservation. They are supplemented with individual species conservation equations and equations for vibrational energy conservation for molecular components.

The equations derived from the Navier-Stokes equations, are based on the continuum postulate which assumes that within a computational volume, there are a large number of molecules such that the average statistical properties of the molecules correctly represent the properties of the fluid in this elementary volume. For gas flows, the continuum formulation requires that the mean free path of the molecules ($\lambda$) is much shorter than the characteristic length scale ($L$) of the flow field under consideration. The ratio of these length scales is named as Knudsen number ($Kn = \frac{\lambda}{L}$). It can then be shown that the Knudsen number is related to the Mach number ($Ma$) and Reynolds number for high speed flows [120]:

$$Kn \propto \frac{Ma}{\sqrt{Re}}$$

(2.1)

The continuum postulate is considered valid for the values of the Knudsen number lower than 0.02-0.03.

The total energy of a molecule is the sum of its translational, rotational, vibrational, electronic and zero-point energy. For a single atom, only translational and electronic energies exist. The various forms of energy are discussed in section 2.2.1.1. It is assumed that each of the species of the mixture behaves as a perfect gas. The thermal state of the gas is assumed to be described by separate and independent temperatures. The translational-rotational state of the gas is assumed to be characterized by a single temperature $T^{tr}$. This assumption is reasonable at conditions within the continuum regime where, for air species rotational equilibration with translation takes typically five collisions. The energy contained in the vibrational modes of the diatomic species $m$ is assumed to be described by the vibrational temperature $T^{vib}$. The vibrational state is assumed to conform to the harmonic oscillator description at all vibrational temperatures. In this study, the ionization is neglected and only
the chemical and vibrational nonequilibrium phenomena are taken into account. Considering these hypotheses, the air mixture is composed of 5 species ($N_2$, $O_2$, $NO$, $N$, $O$), where $N_2$, $O_2$ and $NO$ are in vibrational nonequilibrium.

At high temperatures, molecular collisions result in the exchange of the translational, rotational, vibrational, and electronic energies with the collision partners. The probabilities of these elementary processes differ significantly, giving rise to widely separate relaxation times for the internal modes. Thus, it becomes important to account for the rates of relaxation processes to predict the nonequilibrium behavior. The disparate eigenvalues of these relaxation times have significant physical and computational implications. These energy exchange processes are discussed in section 2.2.4.

Accurate computations in the time scales of the kinetic processes in transatmospheric flow-fields require knowledge of the reaction processes’s finite rates. The proper treatment of energy transfers between nonequilibrium molecular energy modes and the dissociation and ionization processes has important implications in the accurate prediction of the aerodynamic heating on hypersonic vehicles and thrust in propulsive nozzles. In turn, nonequilibrium vibrational energy distributions are required for prediction of dissociation rates, interpretation of radiation experiments, and interpretation of ionic recombination. In section 2.2.3, the coupling between vibration and dissociation is discussed.

2.1 Governing equations

Species conservation:
The mass conservation equation for species $c_k$ in the mixture is governed by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho y) = \frac{\partial}{\partial t} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = \frac{\partial}{\partial y} (\rho y) = \frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho v) + \frac{\partial}{\partial y} (\rho w) = 0 \tag{2.2}$$

In the above equation, the term (1) represents the rate of change of mass of species $c_k$ per unit volume in a cell centered at point $(x,y)$. In term (2), $\rho u$ represents the $x$-component of flux of mass of species $c_k$ convected across cell walls and $\rho v$ is the $y$-component of species diffusion flux across cell walls. Term (3) has the same meaning as term (2) but in the $y$-direction. Term (4) represents the mass production rate of species $c_k$ due to chemical reactions. Clearly $\sum_{n=1}^{N_s} \delta_{c} = 0$, since mass is conserved in chemical changes. The diffusion flux $\delta_{c}^{ij}$ is discussed in section 2.3.1. The composition of $\delta_{c}$ is the subject of section 2.2.2.

Global continuity:
The total mass conservation for the mixture as a whole is given by summing the $N_s$ individual species mass conservation equations. The global continuity equation is written as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho y) = 0 \tag{2.3}$$
In the above equation, term (1) is the rate of change of mass of the mixture per unit volume in a cell centered at \((x,y)\). Terms (2) and (3) are \(x\) and \(y\) components of the mass flux. The global continuity equation is an auxiliary specification that can be used as a numerical check in CFD. The other way to make use of this specification in CFD formulation is to use this together with mass conservation equations for \(N_g = 1\) species. This option is an elegant way in the case, where a CFD code written for ideal gas is being extended to take into account chemical reactions.

**Global momentum conservation:**
The momentum balance for the mixture is given by

\[
\frac{\partial \rho u_{x}}{\partial x} + \frac{\partial (\rho u_{x}^2 + p - \tau_{xx})}{\partial x} + \frac{\partial (\rho u_{y} - \tau_{xy})}{\partial y} = 0 \quad (2.4)
\]

\[
\frac{\partial \rho u_{y}}{\partial y} + \frac{\partial (\rho u_{y}^2 + p - \tau_{xy})}{\partial x} + \frac{\partial (\rho u_{x} + p - \tau_{yy})}{\partial y} = 0 \quad (2.5)
\]

In Eq. (2.4), term (1) is the rate of change of \(x\) component of momentum per unit volume in a cell centered at point \((x,y)\). In term (2), \(\rho u_{x}^2\) is the flux of \(x\) component of momentum convected across cell walls, \(p\) is the pressure forces acting on the cell walls in the \(x\) direction and \(\tau_{xx}\) is the viscous forces acting on cell walls in the \(x\) direction. Term (3) has the same meaning as term (2) but in the \(y\) direction. The terms appearing in Eq. (2.5) have the similar meaning as in Eq. (2.4).

**Vibrational energy conservation:**
Vibrational energy conservation is a phenomenological description of the average energy in the vibrational mode for each molecular species. The conservation of vibrational energy is governed by

\[
\frac{\partial \rho \phi_{m}(^{\text{rot}}T_{m})}{\partial t} + \frac{\partial (\rho \phi_{m}(^{\text{rot}}T_{m}) (u - v_{rot}))}{\partial x} + \frac{\partial (\rho \phi_{m}(^{\text{rot}}T_{m}) (v - v_{rot}))}{\partial y} = \Omega_{m} \quad (2.6)
\]

In the above equation, term (1) represents the rate of change of vibrational energy of molecule \(m\) per unit volume in a cell centered at \((x,y)\). In term (2), \(\rho \phi_{m}(^{\text{rot}}T_{m}) (u - v_{rot})\) is the \(x\) component of the flux of vibrational energy convected across cell walls. \(v_{rot}\), which is discussed in section 2.3.3, consists of two parts: the first part is the conduction of vibrational energy across cell walls due to vibrational temperature gradients in the \(x\) direction and the second part is the diffusion of vibrational energy across cell walls due to molecular concentration gradients in the \(x\) direction. Term (3) has the same meaning as term (2) but in the \(y\) direction. Term (4) represents the source term arising out of various energy exchange processes and is expressed as

\[
\Omega_{m} = \Omega_{\text{v}T} + \Omega_{\text{VT}} + \Omega_{\text{VT}T}, \quad (2.7)
\]

where \(\Omega_{\text{v}T}\) is the vibrational energy lost or gained due to molecular depletion (dissociation) or production (recombination) in the cell, \(\Omega_{\text{VT}}\) is the energy exchange between vibrational and translational modes due to collisions within the cell, and \(\Omega_{\text{VT}T}\) is the energy exchange between vibrational modes
of molecule \( m \) with different molecules. The various energy exchange processes are discussed in sections 2.2.3 and 2.2.4.

**Total energy conservation:**
The conservation of total energy (internal + kinetic) is governed by

\[
\frac{\partial {\hat H}}{\partial t} + \frac{\partial}{\partial x} ((\rho{\hat E} + p)u - (\tau_{xx} + v\tau_{xy} + q_{bx})) + \frac{\partial}{\partial y} ((\rho{\hat E} + p)v - (\tau_{yx} + v\tau_{yy} + q_{by})) = 0
\]

(2.8)

In the above equation, term (1) is the rate of change of total energy per unit volume in a cell centered at \((x,y)\). In term (2), \((\rho{\hat E} + p)u\) is the \( x \) component of total enthalpy flux convected across cell walls, \(\tau_{xx} + v\tau_{xy}\) is the work done by shear forces. \(q_{bx}\), which is discussed in section 2.3.3, consists of two parts: the first part is the conduction of thermal energy across cell walls due to temperature gradients in the \( x \) direction and the second part is the diffusion of enthalpy across cell walls due to concentration gradients in the \( x \) direction. Term (3) has the same meaning as term (2) but in the \( y \) direction.

The governing equations for flows in thermochemical nonequilibrium can be written in a form suitable for numerical formulation as follows:

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial x} (\mathbf{F}_{\text{inv}} - \mathbf{F}_{\text{visc}}) + \frac{\partial}{\partial y} (\mathbf{G}_{\text{inv}} - \mathbf{G}_{\text{visc}}) = \mathbf{S},
\]

(2.9)

where \( \mathbf{U} \) is the vector of conserved quantities. The vectors \( \mathbf{F}_{\text{inv}}, \mathbf{G}_{\text{inv}} \) are the inviscid fluxes and \( \mathbf{F}_{\text{visc}}, \mathbf{G}_{\text{visc}} \) are the viscous fluxes of the conserved quantities in the \( x \) and \( y \) directions, respectively. \( \mathbf{S} \) is the vector of source terms arising out of physiochemical processes. These vectors are given by

\[
\mathbf{U} = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho e \\
\rho e^{(\text{visc})} \\
\rho e^{(\text{phys})} \\
\rho E
\end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix}
\dot{\rho} \\
0 \\
\dot{\rho} u \\
0 \\
\dot{\rho} v \\
0 \\
\dot{\rho} E
\end{bmatrix}
\]

(2.10)
2.1 Governing equations

\[
F_{\text{En}} = \begin{bmatrix}
\rho u \\
\cdot \\
\cdot \\
\rho u
\end{bmatrix}

, \quad G_{\text{En}} = \begin{bmatrix}
\rho v \\
\cdot \\
\cdot \\
\rho v
\end{bmatrix}
\]

\[
F_{\text{Vs}} = \begin{bmatrix}
-\frac{\partial P}{\partial x} \\
\cdot \\
\cdot \\
\cdot \\
0
\end{bmatrix}

, \quad G_{\text{Vs}} = \begin{bmatrix}
-\frac{\partial P}{\partial y} \\
\cdot \\
\cdot \\
\cdot \\
0
\end{bmatrix}
\]

\[
F_{\text{Vb}} = \begin{bmatrix}
\tau_{xx} \\
\tau_{xy} \\
\cdot \\
\cdot \\
u \tau_{xx} \cdot v \tau_{xy} + q_x
\end{bmatrix}

, \quad G_{\text{Vb}} = \begin{bmatrix}
\tau_{xy} \\
\tau_{yy} \\
\cdot \\
\cdot \\
\cdot \\
u \tau_{xy} \cdot v \tau_{yy} + q_y
\end{bmatrix}
\]

The viscous stresses can be written for a Newtonian fluid as

\[
\tau_{xx} = \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)
\]

(2.13)

\[
\tau_{xy} = \frac{2}{3} \mu \left( \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right)
\]

(2.14)

\[
\tau_{yy} = \mu \left( \frac{\partial v}{\partial y} + \frac{\partial v}{\partial x} \right)
\]

(2.15)

The total energy \( E \) per unit mass, being the sum of the internal and kinetic energies, is defined as

\[
E = \frac{1}{2} (u^2 + v^2) + \epsilon
\]

(2.16)

where \( \epsilon \) is the internal energy per unit mass of the gas mixture and \( u, v \) are the velocity components in the \( x, y \) directions, respectively.
2.2 Thermochemical modelling

2.2.1 Thermodynamic relations

An essential ingredient of any high-temperature flow-field analysis is the knowledge of the thermo-
dynamic properties of the gas. To compute aerothermodynamic flow fields accurately, the energy
contained in a molecule and the derived quantities such as specific heat, enthalpy and entropy have
to be known for the appropriate range of temperatures. The methods of statistical mechanics provide
a quick and accurate way of calculating equilibrium thermodynamic properties of high-temperature
gases.

2.2.1.1 Different forms of energy

The internal specific energy of a molecular component is given by

$$\epsilon_{\text{m}} = \epsilon_{\text{m}}^{(p)} + \epsilon_{\text{m}}^{(a)} \tag{2.17}$$

The extent to which the energy may be broken down into independent kinds depends on the accuracy
required. For gases with weakly interacting particles, the separation into a translational energy $\epsilon_{\text{m}}^{(p)}$
and an internal energy $\epsilon_{\text{m}}^{(a)}$ is completely appropriate. For most engineering purposes $\epsilon_{\text{m}}^{(a)}$ can be
written as follows:

$$\epsilon_{\text{m}}^{(a)} = \epsilon_{\text{m}}^{(o)} + \epsilon_{\text{m}}^{(v)} + \epsilon_{\text{m}}^{(b)} + \epsilon_{\text{m}}^{(0)} \tag{2.18}$$

where the last three terms are identically zero for atomic components. The zero point energy of a
molecular component is taken to be equal to the dissociation energy of the molecule at ground state.
For temperatures of interest in gasdynamic problems, the energy of the molecules is distributed over
so many energy levels, that a Boltzmann distribution of the molecules over the energy levels can be
assumed. A Boltzmann distribution for a system of $N$ molecules in thermodynamic equilibrium has the form \([109]\]

$$N_j = N g_j e^{-\frac{\epsilon_j}{kT}} Q, \tag{2.19}$$

where $N_j$ is the number of molecules in a given energy level $\epsilon_j$, $g_j$ is the degeneracy of the level $j$,
and $k$ denotes the Boltzmann constant. The partition function $Q$ is defined as

$$Q = \sum_j g_j e^{\frac{-\epsilon_j}{kT}} \tag{2.20}$$

The average energy in energy mode $i$ per unit mass of species $\epsilon_\alpha$ can be written as

$$\epsilon_{\text{m}}^{(i)} = R_\alpha T^2 \left( \frac{\partial \ln Q_{\text{m}}(\epsilon)}{\partial T} \right) \tag{2.21}$$
2.2 Thermochemical modelling

The corresponding specific heat capacity at constant volume \( c_{v,\alpha}^{(\text{rot})} \) is given as

\[
\frac{c_{v,\alpha}^{(\text{rot})}}{N_\Lambda} = \left( \frac{\partial (\bar{u}^{(\text{rot})})}{\partial T} \right)
\]  

(2.22)

Translation

For weakly interacting particles, the following relations are obtained for the translational mode of energy [55], [109]:

\[
Q_{\alpha}^{(\text{tr})} = \left( \frac{2\pi M_{\alpha} k T}{N_\Lambda h^2} \right)^{3/2} V
\]  

(2.23)

\[
\epsilon_{\alpha}^{(\text{tr})} = \frac{3}{2} R_\alpha T
\]  

(2.24)

\[
\phi_{\alpha}^{(\text{tr})} = \frac{3}{2} R_\alpha
\]  

(2.25)

Rotation

At sufficiently high temperatures, the following relations are obtained for rotational mode of energy [55], [109]:

\[
Q_{\alpha}^{(\text{rot})} = \frac{1}{N_\Lambda h_\alpha^{(\text{rot})}} T
\]  

(2.26)

\[
\epsilon_{\alpha}^{(\text{rot})} = R_\alpha T
\]  

(2.27)

\[
\phi_{\alpha}^{(\text{rot})} = R_\alpha
\]  

(2.28)

where \( \Lambda \) is a symmetry factor that is 2 for homonuclear and 1 for heteronuclear molecules. The characteristic temperature for rotation is expressed in terms of moment of inertia \( I \) of the molecule as follows:

\[
\phi_{\alpha}^{(\text{rot})} = \frac{I^2}{8k_\text{B}R_\alpha}
\]  

(2.29)

Vibration

For a harmonic oscillator of frequency \( \nu \), the following relations are obtained [109]:

\[
Q_{\alpha}^{(\nu)} = \frac{1}{1 - e^{-\nu T}}
\]  

(2.30)

\[
\epsilon_{\alpha}^{(\nu)} = \frac{R_\alpha}{e^{\nu T} - 1}
\]  

(2.31)

\[
\phi_{\alpha}^{(\nu)} = \frac{R_\alpha (\nu T)^2}{(e^{\nu T} - 1)^2}
\]  

(2.32)

The above relations are derived considering infinite number of vibrational energy states. At temperatures, sufficiently high that dissociation occurs, the number of vibrational states is taken to be finite and the upper vibrational level is taken to be corresponding to dissociation energy. In this case the
following relations are obtained [55]:

\[
Q^{(\text{vib})}_{\alpha} = \frac{1 - e^{-\theta^{(\text{vib})}_{\alpha}/T}}{1 - e^{-\theta^{(\text{vib})}_{\alpha}/T}}
\]  
(2.33)

\[
\epsilon^{(\text{vib})}_{\alpha} = \frac{R_{\alpha} (\theta^{(\text{vib})}_{\alpha}/T)}{e^{\theta^{(\text{vib})}_{\alpha}/T} - 1} - \frac{R_{\alpha} (\theta^{(\text{vib})}_{\alpha}/T)}{e^{\theta^{(\text{vib})}_{\alpha}/T} - 1}
\]  
(2.34)

\[
\epsilon^{(\text{vib})}_{\text{gas}} = \frac{R_{\alpha} (\theta^{(\text{vib})}_{\alpha}/T)^2 e^{\theta^{(\text{vib})}_{\alpha}/T}}{(e^{\theta^{(\text{vib})}_{\alpha}/T} - 1)^2} - \frac{R_{\alpha} (\theta^{(\text{vib})}_{\alpha}/T)^2 e^{\theta^{(\text{vib})}_{\alpha}/T}}{(e^{\theta^{(\text{vib})}_{\alpha}/T} - 1)^2}
\]  
(2.35)

The characteristic temperature of vibration \(\theta^{(\text{vib})}_{\alpha}\) is given by

\[
\theta^{(\text{vib})}_{\alpha} = \frac{\hbar \nu}{k}
\]  
(2.36)

The values of \(\theta^{(\text{vib})}_{\alpha}\) for different molecular species can be found in Table B.1.

**Electronic excitation**

In order to evaluate the electronic partition function, no close-form expression can be found. The following relations are used for electronic excitations [55]:

\[
Q^{(\text{e})}_{\alpha} = \sum_{i=0}^{I_{\text{e}}} \frac{c_{\text{e},i}^{(\text{e})} e^{-\theta^{(\text{e})}_{\alpha}/T}}{c_{\text{e},i}^{(\text{e})}}
\]  
(2.37)

\[
\epsilon^{(\text{e})}_{\alpha} = \frac{R_{\alpha}}{c_{\text{e},i}^{(\text{e})}} \sum_{i=0}^{I_{\text{e}}} c_{\text{e},i}^{(\text{e})} \theta^{(\text{e})}_{\alpha} e^{-\theta^{(\text{e})}_{\alpha}/T}
\]  
(2.38)

\[
\epsilon^{(\text{e})}_{\text{gas}} = \frac{R_{\alpha}}{T^2} \left( \sum_{i=0}^{I_{\text{e}}} \frac{c_{\text{e},i}^{(\text{e})}}{c_{\text{e},i}^{(\text{e})}} \theta^{(\text{e})}_{\alpha} e^{-\theta^{(\text{e})}_{\alpha}/T} - \frac{\epsilon^{(\text{e})}_{\alpha}}{R_{\alpha}} \right)
\]  
(2.39)

**Zero point energy**

Since the zero point energy is constant, the following relations are obtained for it [55]:

\[
Q^{(0)}_{\alpha} = \epsilon^{(0)}_{\text{gas}}
\]  
(2.40)

\[
\epsilon^{(0)}_{\alpha} = -R_{\alpha} \epsilon^{(0)}_{\text{gas}}
\]  
(2.41)

\[
\epsilon^{(0)}_{\text{gas}} = 0
\]  
(2.42)

The specific heat capacity at constant volume for a component is given by

\[
\epsilon_{\text{v},\alpha} = \epsilon^{(p)}_{\text{v},\alpha} + \epsilon^{(\text{vib})}_{\text{v},\alpha} + \epsilon^{(\text{e})}_{\text{v},\alpha}
\]  
(2.43)

The specific heat capacity at constant pressure for a component is defined as

\[
C_{\text{p},\alpha} = \left( \frac{\partial h_{\alpha}}{\partial T} \right)
\]  
(2.44)
2.2 Thermochemical modelling

where \( h_{\alpha} \) is the enthalpy per unit mass of the species \( \alpha \) and is given as

\[
h_{\alpha} = c_{\alpha} + \frac{P_{\alpha}}{\rho_{\alpha}}
\]  \hspace{1cm} (2.45)

Assuming that each species behaves as a thermally perfect gas and obey the perfect gas equation, the partial pressure of the species \( \alpha \) is given by

\[
p_{\alpha} = \rho_{\alpha} R_{\alpha} T
\]  \hspace{1cm} (2.46)

Using the above equation, \( c_{p\alpha} \) can be expressed as

\[
c_{p\alpha} = c_{v\alpha} + R_{\alpha} = c_{v\alpha} + \frac{R_{\alpha}}{M_{\alpha}}
\]  \hspace{1cm} (2.47)

2.2.1.2 Mixture properties

The mixture density \( \rho \) and mixture pressure \( p \) can be found by summing over the partial densities and partial pressures of all species, respectively:

\[
\rho = \sum_{\alpha=1}^{N_{\alpha}} \rho_{\alpha}
\]  \hspace{1cm} (2.48)

\[
p = \rho R_{\alpha} T^{(tr)} \sum_{\alpha=1}^{N_{\alpha}} X_{\alpha}/M_{\alpha},
\]  \hspace{1cm} (2.49)

where \( X_{\alpha} = \rho_{\alpha}/\rho \) is the mass fraction and \( M_{\alpha} \) is the molar weight of the species \( \alpha \), respectively. \( R_{\alpha} \) is the universal gas constant and \( T^{(tr)} \) is the translation temperature. Here, a common temperature is assigned to all translational, rotational and electronic modes. Independent temperatures \( T^{(rot)}_{N_{\alpha}^{(a)}} \) and \( T^{(vib)}_{N_{\alpha}^{(a)}} \) are introduced for the vibrational modes of the molecular components. If flows in thermal equilibrium are considered, in numerical simulations a common temperature \( T \) is assigned to all modes. The pressure is only a function of the translational temperature, since only the translational part of the energy effects the pressure [109].

The total energy \( E \) per unit mass, being the sum of kinetic and internal energies, is defined as

\[
E = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) + \sum_{\alpha} X_{\alpha} c_{v\alpha}
\]  \hspace{1cm} (2.50)

where \( c_{v\alpha} \) is the total specific energy per unit mass of the species \( \alpha \), as defined in eq. 2.17 and \( \dot{x}, \dot{y} \) are the velocity components in \( x, y \) directions, respectively.

The specific heat capacities of the mixture are given by

\[
c_{v} = \sum_{\alpha} X_{\alpha} c_{v\alpha}
\]  \hspace{1cm} (2.51)

\[
c_{p} = \sum_{\alpha} X_{\alpha} c_{p\alpha} = c_{v} + R_{\alpha} \sum_{\alpha} \frac{X_{\alpha}}{M_{\alpha}}
\]  \hspace{1cm} (2.52)
The ratio of specific heats \( \gamma \) is given by

\[
\gamma = \frac{C_v}{C_l} = 1 + \frac{P}{\rho} \sum_{\alpha} \frac{X_\alpha}{M_\alpha}
\]  
(2.53)

The total enthalpy per unit mass is defined by

\[
H = E + \frac{P}{\rho}
\]  
(2.54)

The calculation of \( \epsilon_{\alpha} \) using the relations given above is very expensive. The use of curve-fits is an economical way, since it makes fast calculation of \( \epsilon_{\alpha} \) and \( c_{\alpha r} \). In this work, the curve-fits developed by Klomfaß [55], [56] are used.

### 2.2.2 Chemical kinetic model

The chemical source terms are derived from the reactions that occur between the components of the gas. As reactions occur, a mass transfer process between species takes place. This is represented by the term \( \dot{\eta}_{\alpha} \) on the right hand side of the species conservation equation, Eq. 2.2. In this section, the expressions for these mass transfer rates are derived.

A number of different elementary chemical reactions between species in the gas can occur simultaneously. Consider the \( r \)th chemical reaction of \( N_e \) elementary reactions between \( N_e \) chemically reacting species:

\[
\sum_{\alpha=1}^{N_e} \dot{\eta}_{\alpha} \chi_\alpha = \sum_{\alpha=1}^{N_e} \dot{\eta}_{\alpha}' \chi_\alpha
\]  
(2.55)

where \( \dot{\eta}_{\alpha}' \) and \( \dot{\eta}_{\alpha} \) represent the stoichiometric mole numbers of reactants and products of reaction \( r \), respectively and \( \chi_\alpha \) is the molar concentration of the species \( \alpha \). The chemical reaction equation, eq. 2.55 consists of a forward and backward part. The forward and backward reaction rates are given by

**forward:**

\[
\frac{d\chi_{\alpha}}{dt} = (\dot{\eta}_{\alpha}' - \dot{\eta}_{\alpha}) \left[ \frac{k_{fr} \prod_{c=1}^{N_e} [\chi_{\alpha}^{\gamma_{\alpha c}'}]}{\prod_{c=1}^{N_e} [\chi_{\alpha}^{\gamma_{\alpha c}''}]} \right],
\]  
(2.56)

**backward:**

\[
\frac{d\chi_{\alpha}}{dt} = (\dot{\eta}_{\alpha}' - \dot{\eta}_{\alpha}) \left[ \frac{k_{br} \prod_{c=1}^{N_e} [\chi_{\alpha}^{\gamma_{\alpha c}''}]}{\prod_{c=1}^{N_e} [\chi_{\alpha}^{\gamma_{\alpha c}'}]} \right],
\]  
(2.57)

where \( k_{fr} \) and \( k_{br} \) are respectively the forward and backward reaction rate coefficients of reaction \( r \), which generally depend on a reaction temperature. The net rate for the above general reaction \( r \) can be written as

\[
\frac{d\chi_{\alpha}}{dt} = \frac{d\chi_{\alpha}^f}{dt} - \frac{d\chi_{\alpha}^b}{dt} = (\dot{\eta}_{\alpha}' - \dot{\eta}_{\alpha}) \left[ k_{fr} \prod_{c=1}^{N_e} [\chi_{\alpha}^{\gamma_{\alpha c}'}] - k_{br} \prod_{c=1}^{N_e} [\chi_{\alpha}^{\gamma_{\alpha c}''}] \right]
\]  
(2.58)

The above equation is a general form of law of mass action, which ensures the preservation of total mass during a chemical reaction.
2.2 Thermochemical modelling

The mass rate of production of species \( \alpha \) per unit volume is expressed as

\[
\Delta n_\alpha = \frac{d}{dt} (\rho_\alpha) = M_\alpha \sum_{r=1}^{N_R} \frac{d}{dt \rho_{\alpha r}}
\]  

(2.59)

A chemical kinetic model is defined when a set of \( N_R \) reactions is provided with the appropriate expressions for the forward and backward rate coefficients. The forward reaction rates are generally determined experimentally. The empirical relations for many reactions can be correlated in the form

\[
k_{\text{fr}} = \frac{-E_{\text{fr}}}{C_{\text{fr}} T_{\text{fr}}^{n_{\text{fr}}} e^{-E_{\text{fr}}/T_{\text{fr}}}}
\]  

(2.60)

where \( E_{\text{fr}} \) is the activation energy and \( C_{\text{fr}} \) is a constant. Equation 2.60 is known as the Arrhenius equation. The parameters \( C_{\text{fr}}, n_{\text{fr}} \) and the activation energy \( E_{\text{fr}} \) for different reactions are found from experimental data. Under the usual assumptions, the backward reaction rate coefficients are given by [109]

\[
k_{\text{br}} = \frac{k_{\text{fr}} (K_{\text{eqr}})}{K_{\text{eqr}} (T_{\text{eqr}})}
\]  

(2.61)

where \( K_{\text{eqr}} \) is the equilibrium constant for the \( r \)th reaction. The equilibrium constant can be determined from the activation energy of the forward reaction and the partition functions of the reactants and products [109]. In the present work, the curve fit developed by Klomfaß [55], [56] was employed to determine the equilibrium constant.

In the present work, a five component air model consisting of species \( N_2, O_2, NO, N \) and \( O \) is considered. The most important chemical reactions between these species are

\[
N_2 + M \rightleftharpoons 2N + M
\]  

(2.62)

\[
O_2 + M \rightleftharpoons 2O + M
\]  

(2.63)

\[
NO + M \rightleftharpoons N + O + M
\]  

(2.64)

\[
NO + O \rightleftharpoons N + O_2
\]  

(2.65)

\[
N_2 + O \rightleftharpoons NO + N
\]  

(2.66)

where \( M \) represents a generic particle that acts as a collision partner in the reaction and is not altered. The first three are dissociation reactions and the last two are bimolecular exchange reactions (sometimes called the “shuffle reactions”). The exchange reactions are the two most important reactions for the formation of nitric oxide, \( NO \) in air. While deriving the chemical source term according to eq. 2.59, it should be noted that the sum of the mass transfer rates is identically zero and that elemental conservation holds, as required. The application of elemental conservation provides the two additional equations:

\[
\rho_N + \rho_O \rightleftharpoons \frac{M_N}{M_{NO}} \rho_{NO} \quad \text{const}.
\]  

(2.67)

\[
\rho_O + \rho_N \rightleftharpoons \frac{M_O}{M_{NO}} \rho_{NO} \quad \text{const}.
\]  

(2.68)
With these two equations, the system of equations to determine the chemical source term become overdetermined. In general, numerical methods are very sensitive to any disturbance of elemental conservation. Thus to guarantee the elemental conservation, the mass production rates of molecular components are determined using eq. 2.59 and for atomic components, eqs. 2.67-2.68 are used. The magnitudes of the published reaction rate coefficients vary greatly, especially at high temperatures. In the context of the present work, five different chemical kinetic models are used [24], [38], [79], [80], [81]. The parameters associated with the rate coefficients are given in Appendix A. Figures 2.1-2.8 show the reaction rate coefficients for the dissociation and exchange reactions. At high temperatures the deviations in rate coefficients are clearly observed for different models. The difference becomes more significant for exchange reactions. In some of the figures, curves representing two or more different chemical models overlap each other, since the reaction rate coefficients for some reactions are same for different chemical models.

The reaction mechanism and their kinetic rates are a source of considerable uncertainty for the air chemistry at high temperatures. Although there is no dearth of data in this regard from shock tube studies, their gross disagreements are well known [91]. Parametric sensitivity studies carried out in the present work using the above mentioned chemical kinetic models and relaxation models for high enthalpy nitrogen flows past a cylinder show that a practical quantity like the shock stand-off distance can be changed by as much as $10\%$ between the extreme cases. Similar findings were also reported by Hannemann [42]. Considering these uncertainties of chemical kinetic models, a least square curve fit has been made of the rates of the above mentioned chemical kinetic models. In this approach the modified Arrhenius equation (eq. 2.60) is used as an ansatz. The new set of rate coefficients ensure that the reaction rates are at a minimal deviation from reaction rates of all the five chemical kinetic models used. The coefficients $C_{fr}$, $\alpha_{fr}$ and $E_{fr}$ thus deduced from this least square curve fit is given in Appendix A, along with the coefficients of other chemical kinetic models. In the Figs. 2.1-2.8, the curvefit represents this new set of reaction rate. In chapter 5, with the help of a computation, the usefulness of this new reaction set will be discussed.

Most of the sources for reaction rate coefficient data have assumed thermal equilibrium and, consequently, provide these expressions as a function of a single temperature. However, under the low density and high energy flow conditions of interest, where thermal equilibrium may not be assumed, the characteristic chemical time scale for dissociative reactions is comparable to the characteristic time for vibrational relaxation, a condition suggesting the coupling between the vibrational and chemical processes. Models for such chemical-vibrational coupling are considered in the next section.

### 2.2.3 Vibration-dissociation coupling

The chemical changes (e.g. dissociation and recombination) in molecules depend on their internal states of motion as well. Only those possessing a total energy above a threshold value are able to activate a chemical change. At high temperatures, the characteristic times for chemical and vibrational relaxation are comparable, leading to a mutual coupling. For example, in the case of the compressive
2.2 Thermochemical modelling

Figure 2.1: Forward rate reaction coefficients for
$N_2 + N_2 \rightarrow 2N + N_2$

Figure 2.2: Forward rate reaction coefficients for
$N_2 + N \rightarrow 2N + N$

Figure 2.3: Forward rate reaction coefficients for
$O_2 + N_2 \rightarrow 2O + N_2$

Figure 2.4: Forward rate reaction coefficients for
$O_2 + N \rightarrow 2O + N$
Figure 2.5: Forward rate reaction coefficients for \( NO + N_2 \rightarrow N + O + N_2 \)

Figure 2.6: Forward rate reaction coefficients for \( NO + N \rightarrow N + O + N \)

Figure 2.7: Reaction rate coefficients for exchange reaction \( NO + O \rightarrow N + O_2 \)

Figure 2.8: Reaction rate coefficients for exchange reaction \( N_2 + O \rightarrow NO + N \)
flow through a shock wave, the vibrational temperature will be lower than the translational-rotational temperature. As the molecules have less vibrational energy than at equilibrium, the nonequilibrium molecular dissociation rate will be lower than the equilibrium dissociation rate. The experimentally measured dissociation rate as reported in the literatures is interpreted to be the equilibrium value; thus the dissociation rate must be modified if there is vibrational nonequilibrium. At the same time, as vibrationally excited molecules are more likely to dissociate, there is a drain on the vibrational energy, which reduces the rate of vibrational relaxation. Hence it is necessary to understand and quantify this interaction, to predict the correct nonequilibrium dissociation rates. These rates have a large impact on macroscopic flow characteristics, such as heating rates and shock shapes. Small differences in the shock shape, and the resulting differences in the pressure field, can lead to large differences in the predicted aerodynamic moments.

Two types of chemical-vibrational coupling have been suggested in the literature. Under the first coupling model, known as preferential dissociation, higher vibrational energy states being the ones preferred for entering into chemical reactions. Molecules in the lower vibrationally excited states must “ladder climb” to the higher vibrationally excited states before dissociation can occur. However, this model may not be valid at very high velocities. Under highly energetic conditions, the ladder climbing process may not be as significant and a second model, based on nonpreferential dissociation may be more realistic [33], [91], because at these conditions the molecules at any vibrational level may have sufficient energy to dissociate.

2.2.3.1 Park model

The simplest, conceptually and in practical implementation, is a model set up by Park based on an analysis of shock tube experimental data on reaction rates [81]. In this model, Park assumes that certain classes of reactions can be described by a single rate-controlling temperature which is an appropriate average of the local translational and vibrational temperatures. He suggests the evaluation of the dissociation rate coefficient \( k_{d} \) at an average temperature \( T_{\text{av}} = T_{\text{tr}} T_{\text{vib}} \), where \( T_{\text{tr}} \) is proposed to be between 0.5 and 0.7. A more recent investigation [91] found that \( n_{1} = \Omega \) gave results for reaction rate coefficients that were within a factor of 3 of those calculated on the basis of the SSH (Schwartz, Slawsky and Herzfeld) theory [92]. Park applies the average temperature relation only in the determination of the forward reaction rate of dissociation reactions. The model assumes that the backward reaction rate is governed by the translational temperature \( T \).

When a molecule dissociates its vibrational energy is lost and conversely in atomic recombination reactions, some energy is put into molecular vibrational modes. These two effects: depletion by dissociation and enhancement by recombination must be accounted for as a source term. Park proposes that molecular dissociation as well as recombination takes place at the vibration temperature \( T_{\text{vib}} \). Therefore, the amount of energy lost or gained due to molecular depletion or production of species \( m \) is given by

\[
\Omega_{T} = \zeta_{m T} \Omega_{T} \tag{2.69}
\]
The justification for Park model lies in its success in prediction of qualitative trends and its simplicity in the implementation of computational fluid dynamics.

### 2.2.3.2 Treanor and Marrone model

The Treanor-Marrone model [69], [102] includes the effect of vibrational relaxation on dissociation through the relation

$$ k_{f_d} = k_{f_d}^* V(T, T_{vn}, U), \quad (2.70) $$

where the vibrational coupling factor $V$ is obtained from

$$ V = \frac{Q(T_{f})Q(T)}{Q(T_{vn})Q(T_{vn})} \quad (2.71) $$

The term $Q$ is the vibrational partition function for the dissociating species and $k_{f_d}^*$ is the dissociation rate constant that would exist under conditions of thermal equilibrium $T_{reac} = T$. The temperature $T_{f}$ is defined as

$$ \frac{1}{T_f} = \frac{1}{T_{vn}} - \frac{1}{T} - \frac{1}{U} \quad (2.72) $$

The probability temperature $U$ models the tendency of the vibrating molecule to dissociate more explicitly at the upper levels (preferential dissociation). $U = \infty$ corresponds to the situation that dissociation occurs with equal probability from any vibrational level in any collision that has sufficient translational energy to effect the dissociation. Treanor and Marrone determined the constant $U$ which best fitted their computations with experiments as $U = \theta_{vn}/3$, where $\theta_{vn}$ is the characteristic dissociation temperature for a dissociation reaction of species $m$.

As in Park model, in this model also the backward reaction rate is governed by the translational temperature $T$. In case of Zeldovich reactions also, the reaction rate is governed by translation temperature.

In Ref. [55], Klomfaß modified the forward reaction rate for all endothermic reactions, according to Treanor and Marrone model. For exothermic exchange reactions, he proposed to modify the reaction rate coefficient by the coupling factor $V$. The argument in favour of such a modification is that the exothermic exchange reactions take place in two steps. In the first step, the endothermic formation of a three body compound $\alpha \rightarrow \beta$ takes place. In the second step, exothermic breaking of atoms of the component $\beta$ and at the same time, formation of molecules of the component $\alpha$ takes place. Since the first step can take place with only for components with sufficient kinetic energy, the modification of the exothermic reaction rate coefficients in case of the exchange reaction is justified. Thus the equation is modified as follows:

$$ k_{f_e} = \frac{k_{f_e}^* V(T, T_{vn}, U)}{k_{eig}} \quad (2.73) $$

Associated with the process of modification of chemical rate coefficients, there is a drain or increment in the vibration energy due to dissociation or recombination. The rate of change of the volume specific
2.2 Thermochemical modelling

vibrational energy as a consequence of dissociation is given by

\[ e^{(dissoci)}_{\text{vib}} = e^{(dissoci)}_{\text{vib}}(T_p) \frac{\partial \mu_{\text{vib}}}{\partial T} \]  

(2.74)

The vibrational energy \( e^{(dissoci)}_{\text{vib}} \) of a dissociating molecule is expressed as

\[ e^{(dissoci)}_{\text{vib}} = e_{\text{vib}}(T_p) \]  

(2.75)

As a consequence of a detailed balance at thermodynamic equilibrium \((T_{\text{vib}} = T)\), the vibrational energy of a molecule after recombination equals that of the dissociating molecule before dissociation.

\[ [e^{(created)}_{\text{vib}}] = [e^{(dissoci)}_{\text{vib}}(T, T_{\text{vib}})]_{eq} = [e^{(dissoci)}_{\text{vib}}(T, T)]_{eq} = e_{\text{vib}}(-U) \]  

(2.76)

If the reaction rate coefficient of the exothermic exchange reaction is modified as proposed in eq. 2.73, then the energy depletion or formation is also considered for molecules participating in exchange reactions.

Formally, the negative quantity \(-U\) in eq. 2.76 may be considered as the temperature at which the molecules are formed by recombination. The negative value relates to the fact that, on the basis of an exponential distribution, more molecules are formed in upper vibrational levels than in lower levels.

In the case of nonpreferential model, \((U = \infty)\), \(T_p = \infty\) for \(T_{\text{vib}} = T\). That means, molecules which are produced due to recombination possess infinite energy. The energy of a molecule produced out of recombination in such a case is given by

\[ e_{\text{vib}}(T_p) = \lim_{T_p \to \infty} e_{\text{vib}}(T_p) = \frac{1}{2} h \nu \left( \epsilon_{\text{vib}}^{(0)} - e^{(dissoci)}_{\text{vib}} \right) \]  

(2.77)

In the limiting case \(T_p = \infty\), the existing Boltzmann distribution is given by

\[ \lim_{T_p \to \infty} \frac{N(T_p)}{N_{\text{vib}}} = \frac{1}{L_{\text{vib}}} \]  

(2.78)

where \(L_{\text{vib}}\) is the maximum number of vibrational states to be considered. This expression interprets that the molecules which are produced as a consequence of recombination follow a statistical distribution and the probability for them to occupy a vibrational level is equal. This model is named as Random recombination model [55].

2.2.4 Relaxation processes

The energy exchange mechanisms between translation and vibrational energy modes due to elastic and inelastic collisions of particles are discussed in this section. The proposed models are simplifications of the complicated energy exchange processes that occur at the molecular level. The following energy exchange processes are discussed:

- vibrational-translational energy exchange (V-T)
- vibrational-vibrational energy exchange (V-V)
2.2.4.1 Vibrational-translational energy exchange

The model of vibrational-translational relaxation is based on the early model of Landau and Teller [61]. The model of Landau and Teller supposes that vibrationally excited diatomic molecules are submerged in an environment (heat bath) consisting of molecules in thermal equilibrium at translational-rotational-vibrational temperature $T$. Such a heat bath can be provided, for example, by a large number of inert gas containing a small concentration of the diatomic species. It can also be provided by the translational and rotational degrees of freedom of a pure diatomic species itself, if only a small fraction of the molecules are excited. The submerged vibrationally excited molecules have a higher vibrational temperature; if only a small fraction of the molecules are excited. The submerged vibrationally excited molecules will exchange their vibrational energy with the translational-rotational energy and after a period of time, will relax towards a new translational-rotational-vibrational equilibrium temperature $T$ of the whole system. This results in a redistribution of internal energy and therefore equilibrium temperature increases. The model is derived for diatomic molecules which are assumed to behave as harmonic oscillators, allowing only transitions by one vibrational quantum level [109]. The resulting vibrational-translational energy exchange rate becomes

$$\Omega_{HT} = \rho_n \frac{c_{\text{vib}}^n(T) - c_{\text{vib}}(T_{\text{heat}})}{\tau_{m}} \, ,$$

(2.79)

where $c_{\text{vib}}^n(T)$ is the vibrational energy per unit mass of the vibrational species $n$ evaluated at the local equilibrium thermodynamic temperature of the heat bath $T$. If, in a general case, the heat bath is not in thermal equilibrium, the local equilibrium thermodynamic temperature is supposed to be equal to the translational-rotational temperature. The quantity $\tau_{m}$ is the molar averaged relaxation time of species $m$ and given as follows [42], [55]:

$$\frac{1}{\tau_{m}} = \sum_n \frac{1}{\tau_{mn}} \, ,$$

(2.80)

where $\tau_{mn}$ is inter-species relaxation time and given as follows:

$$\tau_{mn} = \frac{1}{(1 - \exp(-Q_{mn}/T))^\nu \cdot k_{T}^{\nu}} \, ,$$

(2.81)

The velocity-averaged rate constants $k_{\text{v}}^{\nu}$ are given by SSH theory [55], [92] as follows:

$$k_{\text{v}}^{\nu} = \nu \cdot \frac{\sigma_{\text{v}}^{\nu} e^{\nu} \left( \frac{\alpha^{\nu}}{T} + \frac{\beta^{\nu}}{T^2} + \frac{\gamma^{\nu}}{T^3} \right)}{f_{\text{v}}^{\nu}} \, ,$$

(2.82)

Here the parameters $\sigma_{\text{v}}^{\nu}$, $\alpha^{\nu}$, $\beta^{\nu}$ and $\gamma^{\nu}$ are functions of the characteristic vibrational temperatures, the reduced masses, potential parameter and the steric factor. The collision rate $\omega_{\text{tran}}$ appearing in the above expression is given as follows:

$$\omega_{\text{tran}} = (\sigma_{\text{v}})^2 N_A \sqrt{8\pi k_{\text{b}} T \over \mu_{\text{v}}} \, ,$$

(2.83)
where $\mu_{\text{ran}}$ is the reduced mass of the colliding particles $m$ and $n$ and given as follows [55]:

$$\mu_{\text{ran}} = \frac{M_m M_n}{M_m + M_n}$$  \hspace{1cm} (2.84)

One convenient way to express the inter-species relaxation time is as follows:

$$\tau_{\text{ran}} = \frac{R_n T}{(1 - \exp(-\beta_n \sigma_{\text{lim}}/T)) \mu_{\text{ran}}}$$  \hspace{1cm} (2.85)

Theoretical estimation of rate constants and thus inter-species relaxation time is difficult due to insufficient knowledge of various parameters like the steric factors and the potential parameter. Therefore by means of available experimental data, the unknowns in the equation for inter-species relaxation time is eliminated. In the present work, two such possibilities have been used.

(1) Millikan and White [42], [71], [82] derived a correlation for inter-species relaxation times with available experimentally measured relaxation times. The correlation provides an approximation of inter-species relaxation time in dependence of the characteristic vibration temperature and the reduced molar mass $\mu_{\text{ran}}$ of the colliding particles and is given as follows:

$$\tau_{\text{MW}} = \frac{1}{p} \exp \left[ A \left( T^{-1/3} - 0.0084 \right)^{1/4} \right] - 6.894 \text{ Pa s},$$  \hspace{1cm} (2.86)

with $A = 4.7 \times 10^3 \left( \frac{1}{\mu_{\text{ran}} \sigma_{\text{lim}}} \right) ^{1/3}$. For the molar averaged relaxation time $\tau_m$, Lee [90] proposes the following averaging expression:

$$\tau_m = \frac{\sum_n Y_n}{\sum_n \tau_m n}$$  \hspace{1cm} (2.87)

where $Y_n$ is the mole fraction of species $n$.

If expression 2.86 is used in Eq. 2.87, the average relaxation time $\tau_m$ is denoted by $\tau_{m}^{\text{MW}}$, the Millikan and White relaxation time. For high temperatures ($T > 8000$ K), the Landau-Teller expression (Eq. 2.79), used with Millikan and White relaxation time expressed by Eq. 2.86, yields a relaxation rate that is too large, due to an overprediction of the collision cross-section. Therefore, Park [80] corrected the molar averaged Millikan and White relaxation time as follows:

$$\tau_m = \tau_{m}^{\text{MW}} + \tau_{m}^{P}$$  \hspace{1cm} (2.88)

Park has proposed the following expression for the correction term $\tau_{m}^{P}$:

$$\tau_{m}^{P} = \frac{1}{\sigma m \sqrt{n} \tau_{m}^{\text{MW}}},$$  \hspace{1cm} (2.89)

depending on the number density $n_m$, the average molecular velocity $\bar{v}_m$ and the limiting cross-section $\sigma_{\text{lim}}$. The average molecular velocity is given by

$$\bar{v}_m = \left( \frac{8 R_n T}{\pi M_m} \right)^{1/2}$$  \hspace{1cm} (2.90)
The limiting cross section $\sigma_m$ is a measure of the probability for the collision process. Park proposed $\sigma_m$ to be dependent of the temperature as follows:

$$\sigma_m = 10^{-20} \left( \frac{2000 \text{K}}{T} \right)^2$$  \hspace{1cm} (2.91)

This limiting collision cross-section idea was developed from experiments on nitrogen but can be plausibly applied for other diatomic molecules as well [16]. However, at high temperatures, the vibrational ladder climbing process due to heavy particle collisions becomes diffusive in nature [81]. Park proposes an empirical bridging formula between the Landau-Teller and diffusive rates of the form

$$\Omega_{VT} = \rho_m \frac{\epsilon_m^T(T) - \epsilon_m(T_m)}{\tau_m} \frac{T_{shk} - T_{total}}{T_{shk} - T_{total}} \exp \left( \frac{S_m - 1}{T_{shk}} \right), \quad S_m = 3 S_0 \exp \left( \frac{\epsilon_m^{shk}}{T_{shk}} \right)$$  \hspace{1cm} (2.92)

The quantities $T_{shk}$ and $T_{total}$ are the translational-rotational and molecular species vibrational temperatures evaluated just behind the bow shock wave. At low temperatures, the relaxation is governed by the Landau-Teller rate, and at high temperatures, by the slower diffusive rate. It should be noted that such a model requires an iterative adaptation of the a priori unknown temperatures $T_{shk}$ and $T_{total}$ in CFD codes. For complex geometries the procedure could be time consuming.

(2) Klomfaß [55] made a curve fit for rate constants of VT transitions by means of measured experimental relaxation times. In this context, Eq. 2.82 was as used as ansatz. The parameters $\Omega_{VT}^{0.6}$ and $\epsilon_{VT}^{0.6}$ were chosen as free parameters and were adjusted with the method of least square to the measured relaxation time. Analogous to the theory of Landau and Teller, the parameter $\Omega_{VT}^{0.6}$ in Eq. 2.82 was set as zero. The collision rate was calculated uniformly with $\sigma_{m} = 3 \times 10^{-20} \text{m}^2$. The rate constants of VT transitions, for which experimental data are not available (ex. $N_2 - N$), were determined by extrapolation of MW-data for the rate constants of similar transitions:

$$k_m = \left( \frac{\sigma_{m}^{VT}}{\sigma_{m}} \right)_{MW} \bar{k}_{m}$$  \hspace{1cm} (2.93)

The calculated values of the coefficients are given in Table B.2. Using the calculated values of rate constants, the molar averaged vibrational relaxation time and thus energy transfer associated with VT process can be calculated using Eq. 2.79.

2.2.4.2 Vibrational-vibrational energy exchange

In a mixture of species, each diatomic species can be differently excited. In this case, species can exchange their vibrational energy between each other. This transfer of vibrational energy between the different molecules causes the vibrational energy to equalize.

According to Candler [16], the net VV energy transfer associated with the species $\nu_m$ is given by

$$\Omega_{VV} = \sum_{\nu_m} [\Omega_{VV}]_{\nu_m}$$  \hspace{1cm} (2.94)
where the net vibrational energy exchange of species \( m \) per unit time and unit volume as a result of interaction with species \( \eta \) is given by

\[
\dot{Q}_{\text{V,}\eta-m} = \dot{Q}_{\text{V,}\eta} - \dot{Q}_{\text{V,}m},
\]

where \( \dot{Q}_{\text{V,}\eta-m} \) is the rate of vibrational energy transfer per unit volume and per unit time from species \( \eta \) to species \( m \) and is given as follows:

\[
\dot{Q}_{\text{V,}\eta-m} = P_{\eta-m} Z_{\eta-m} \epsilon_{m} \frac{M_{m}}{N_{A}},
\]

where \( P_{\eta-m} \) is the probability of transferring vibrational energy from \( \eta \) to \( m \), \( \frac{M_{m}}{N_{A}} \) is the average vibrational energy per particle of species \( m \) with \( N_{A} \) as Avogadro’s number. The quantity \( Z_{\eta-m} \) is the number of collisions per unit time and volume. From kinetic theory, an expression for \( Z_{\eta-m} \) can be determined [109] as follows:

\[
Z_{\eta-m} = n_{\eta} \sigma_{\eta-m} \sqrt{\frac{8RT_{\eta}}{\pi a_{\eta}}}.
\]

In this expression, \( n_{\eta} \) and \( T_{\eta} \) appear as the number density of species \( \eta \) and \( T_{\eta} \), respectively. Further \( \rho_{\eta-m} \) is the reduced mass, and \( \sigma_{\eta-m} \) is the collision cross section. The collision cross section \( \sigma_{\eta-m} \) can be approximated by the product of the collision diameters, \( d_{\eta}d_{m} \), of species \( \eta \) and \( m \). The collision diameters are given in Table B.1. The probabilities of an exchange have been measured for several different molecules [99] and have been presented in an exponential form by Park and Lee [90]:

\[
P_{N_{2}-NO} = 5.5 \times 10^{-6} \left( \frac{T}{1013} \right)^{2.82},
\]

\[
P_{N_{2}-O_{2}} = 3.0 \times 10^{-6} \left( \frac{T}{1013} \right)^{2.87},
\]

\[
P_{O_{3}-NO} = P_{N_{2}-NO}
\]

The two probabilities \( P_{\eta-m} \) and \( P_{m-n} \) have to be coupled in such a way that the energy transfer \( \dot{Q}_{\text{V,}\eta-m} \) becomes zero as soon as the two vibrational temperatures \( T_{\eta-m} \) and \( T_{m-n} \) become equal. Thus the two probabilities are coupled as follows:

\[
P_{\eta-m} = P_{m-n} \frac{M_{m}}{M_{\eta}} \left( \frac{T_{\eta-m}}{T_{m-n}} \right)^{3/2}.
\]

The influence of this coupling is rather unimportant in the case of air, since the probabilities \( P_{\eta-m} \) are small.

Another model which is derived directly from gas kinetic theory [55], [97] expresses the net vibrational energy exchange of species \( m \) per unit time and unit volume as a result of interaction with species \( \eta \), as follows:

\[
\dot{Q}_{\text{V,}\eta-m} = \rho_{\eta-m} \sigma_{\eta-m} \sqrt{\frac{8RT_{\eta-m}}{\pi a_{\eta}}} \left( \epsilon_{\eta}^{(\text{a})} + R_{\eta}^{(\text{a})} \epsilon_{\eta}^{(\text{a})} \right) \epsilon_{m}^{(\text{b})} \exp \left( \frac{E_{\eta-m}^{(\text{a})}}{RT_{\eta-m}} \right) - \epsilon_{\eta}^{(\text{a})} R_{\eta}^{(\text{a})} \epsilon_{\eta}^{(\text{a})} \epsilon_{m}^{(\text{b})}.
\]
are given by SSH theory \[92\] as follows:

\[
\left[ \dot{Q}_{\text{V,trans}} \right] = -\left[ \dot{Q}_{\text{V,grad}} \right] \frac{T}{\tau_{\text{H}}} / \frac{T_{\text{H}}}{T}
\]  \hspace{1cm} (2.103)

The velocity averaged rate constants \( \dot{Q}_{\text{V,trans}} \) are given by SSH theory \[92\] as follows:

\[
\dot{Q}_{\text{V,trans}} = \sum_{\alpha} \left[ \dot{Q}_{\text{V,grad}} \right] \left( \frac{T}{\tau_{\text{H}}} + \frac{\dot{Q}_{\text{V,grad}}}{T_{\text{H}}} + \frac{\dot{Q}_{\text{V,trans}}}{T_{\text{H}}} \right)
\]  \hspace{1cm} (2.104)

Unlike rate constants for VT transitions, insufficient experimental data are available for VV transitions. Keeping this in view, Klomfaß \[55\] used the following heuristic relation, which accepts relatively fits the few available experimental data:

\[
\dot{Q}_{\text{V,trans}} = \sum_{\alpha} \left[ \dot{Q}_{\text{V,grad}} \right] \exp \left\{ \left( \frac{T_{\text{H}}}{T} - \frac{T_{\text{H}}}{T_{\text{H}}} \right) / T \right\}
\]  \hspace{1cm} (2.105)

### 2.3 Transport phenomena

By transport phenomena, we refer to the physical properties of viscosity, thermal conduction, and diffusion. The essence of molecular transport phenomena in a gas is the random motion of atoms and molecules. When a particle moves from one spatial location to another, it carries with it a certain momentum, energy and mass associated with the particle itself. The transport of this particle momentum, energy, and mass through the gas due to the random particle motion gives rise to the transport phenomena of viscosity, thermal conductivity and diffusion, respectively.

#### 2.3.1 Mass transport - Diffusion

The kinetic gas theory provides the following expression for the diffusion flux of species \( \alpha \) \[5\], \[73\]:

\[
\mathbf{q}_\alpha = \rho \mathbf{V}_\alpha = \frac{\mathbf{D} \mathbf{c}}{\rho} \sum_{\beta} \mathbf{c}_{\beta} M_{\alpha} M_{\beta} \left( \mathbf{\nabla} \frac{c_{\beta}}{c} + \left( \frac{c_{\beta}}{c} \right) \frac{1}{\rho} \mathbf{\nabla} \mathbf{v} \right) - \mathbf{D}_{\alpha} \frac{1}{T} \mathbf{\nabla} T
\]  \hspace{1cm} (2.106)

where \( c \) is the total molar concentration, \( c = \sum_{\beta} c_{\beta} \) of the gas mixture, \( D_{\alpha} \) and \( D_{\alpha}^{\rho} \) are the multi-component and thermal diffusion coefficient, respectively, \( \mathbf{V}_\alpha \) is the diffusion velocity.

While the concentration induced contribution tends to homogenize the mixture, the other contributions tend to separate the components. Pressure diffusion concentrates heavy particles in regions of high pressure and vice versa. As thermal diffusion has a lower order of magnitude, it is neglected. A most often used simplification to the diffusion flux is obtained, when pressure diffusion is neglected and a single diffusion coefficient is introduced. This approximation is known as Fick’s law \[2\]:

\[
\mathbf{q}_\alpha = \rho \mathbf{V}_\alpha = - \mathbf{D} \mathbf{\nabla} \frac{c_{\beta}}{c}
\]  \hspace{1cm} (2.107)

The diffusion coefficient \( D \) is given by assuming a constant Lewis number \( L_e \):

\[
D = \frac{k L_e}{\rho c}
\]  \hspace{1cm} (2.108)

The Lewis number \( L_e \) is the ratio for energy transfer between diffusion and heat conduction. \( L_e \) is taken between 1.0 and 1.4 for neutral species.
2.3 Transport phenomena

2.3.2 Momentum transport - Viscosity

Viscosity in gases arises principally from the molecular diffusion that transports momentum between layers of the flow. The viscosity of each species \( \alpha \) is found using the Blottner viscosity model, which is a curve fit of experimental data, as a function of temperature [6]. The model uses three constants for a curve fit and yields

\[
\mu_{\alpha} = (3 \pi a_{\text{av}}) \left[ (C_{\alpha}) \left( b_{\alpha} \right) + C_{\alpha} \right],
\]

(2.109)

where the constants \( a_{\text{av}}, b_{\alpha}, C_{\alpha} \) are presented in Table B.3. The curve fits for the viscosity are appropriate for temperatures up to 10,000 K and for weak ionization. The region of a flow field where viscous effects are important is in the boundary layer which for most flows is below this temperature and for the cases that have been computed in this study, the flow field is not likely to be ionized. Thus the viscosity formulation is appropriate for the present work.

The mixture viscosity can be calculated from the species viscosities using Wilke’s semi-empirical mixing rule [117]:

\[
\mu = \sum_{\alpha} c_{\alpha} \mu_{\alpha} \sum_{\beta} c_{\beta} \phi_{\alpha \beta},
\]

(2.110)

where \( c_{\alpha} \) is molar concentration and \( \phi_{\alpha \beta} \) is

\[
\phi_{\alpha \beta} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_{\alpha}}{M_{\beta}} \right)^{-\frac{1}{2}} \left[ 1 + \left( \frac{M_{\alpha}}{M_{\beta}} \right)^{\frac{1}{2}} \left( \frac{M_{\beta}}{M_{\alpha}} \right)^{\frac{1}{2}} \right]^{-2}
\]

(2.111)

2.3.3 Energy transport - Heat conduction

In a chemically reacting viscous flow, there is energy transport due to thermal conduction and species diffusion. The energy flux due to thermal conduction and species diffusion occurs when there is temperature gradients and the species concentration gradients, respectively in the flow field. The total heat flux \( q' \) is given by

\[
q' = q_{\text{cond}} + q_{\text{diff}} = \left[ k^{(\text{th})}_{\text{m}} \nabla T + h^{(\text{m})}_{\text{m}} \nabla T_{\text{m}} \right] + \left[ \rho \sum_{\alpha} \mu_{\alpha} \frac{D_{\text{m}} \nabla \chi_{\alpha}}{\rho} \right]
\]

(2.112)

The vibrational energy flux due to thermal conduction and species diffusion is given by:

\[
q^{(\text{vib})}_{\text{m}} = k^{(\text{vib})}_{\text{m}} \nabla T_{\text{m}}^{(\text{vib})} + h^{(\text{m})}_{\text{m}} D_{\text{m}} \nabla \chi_{\text{vib}}
\]

(2.113)

The conductivities \( k^{(\text{th})} \) and \( k^{(\text{vib})} \) are calculated from species viscosities using the Eucken formula [109]:

\[
k^{(\text{th})}_{\alpha} = \mu_{\alpha} \left( \frac{2}{3} \nu_{\text{av}} + \nu_{\text{m}} \right),
\]

(2.114)

\[
k^{(\text{vib})}_{\alpha} = \mu_{\alpha} \nu_{\text{m}}
\]

(2.115)
The total translational and vibrational conductivity of the mixture are then calculated from Wilke’s mixing rule:

\[
k^{(tr)} = \sum_\alpha \frac{G_\alpha^{(tr)}}{\sum_\beta (\gamma_\beta \epsilon_\beta)}
\]

\[
k^{(vb)} = \sum_\alpha \frac{G_\alpha^{(vb)}}{\sum_\beta (\gamma_\beta \epsilon_\beta)}
\]

where \(\phi_{\alpha3}\) is defined in Eq. 2.111 with \(\mu\) replaced by \(k\).
Chapter 3

Numerical method

The resolution of complex aerodynamic phenomena like shock-shock interactions, shock-wave/boundary layer interactions etc., by a numerical scheme, requires a strongly heterogeneous discretization to account for the different scales. A uniform discretization that is determined by the finest scale is not appropriate, since it requires a prohibitive amount of memory resources and computational time. Memory resources and computational time become very important when a flow field with thermochemical nonequilibrium is analysed. Therefore algorithms have to be developed with computational effort and memory requirements that are proportional to the complexity of the underlying problem, i.e., only in regions where small-scales physical effects are present, the discretization has to be refined, and elsewhere a much coarser discretization will be sufficient. This task can be addressed adequately by locally adaptive schemes. Adaptive methods efficiently utilize available resources and may provide more accurate and reliable solutions. Further, the grid generation process is greatly facilitated, since the initial-coarse-mesh has solely to be adjusted to the geometry but not to the flow solution. Efficient and reliable adaptive strategies require an integrated framework consisting of the components: grid generation, adaptation and flow solver.

In this study, the numerical method used to calculate the approximate solutions to the two-dimensional Euler and Navier-Stokes equations is based on the adaptive code QUADFLOW, being developed at RWTH Aachen. References [12], [13], [14] describe the detailed features of the QUADFLOW code. The method consists of an integrated framework, including a novel grid generation technique using B-Splines to construct meshes with quadrilateral cells in 2D and hexahedral cells in 3D, advanced adaptation criteria based on multiscale analysis and a flow solver which is capable to operate on arbitrary unstructured meshes. In its basic form, the flow solver assumes a thermally and calorically perfect gas model. In the framework of the present study, the QUADFLOW code has been extended to take into account real gas effects typical for hypersonic flow.
3.1 Grid generation

The grid generation is based on a B-Spline technique [9], [10], which is particularly suited for adaptive algorithms, since it provides a very efficient way to represent the mesh at low memory costs. This technique provides excellent adaptability to boundaries. Each block of the mesh is represented by a B-Spline function of the form

$$ x(s) = \sum_i P_i \prod_{k=1}^{d} N_{i}^{(d)}(s_k) , $$

(3.1)

where $P_i$ represents the control points and $d$ denotes the dimension of the space. The order $m$ of the B-Spline function $N^{(d)}$ is chosen as 4. The grid is stored as a function, and therefore only a few control points are required to represent each block. Geometric quantities required by the flow solver may consistently be evaluated at any location within the domain. In particular, a truly nested sequence of locally adapted cells can be provided, which is required by the applied adaptation criteria, based on multiscale analysis. The B-Spline approach can be combined with various grid generation techniques, e.g. algebraic, elliptic or hyperbolic grid generation methods, by means of B-Spline interpolation and approximation. Further details are given in references [8], [9], [10], [11], [12], [13], [14].

The computational domain is initially tessellated by a coarse multiblock structured grid. As basic element types, quadrilaterals and hexahedra are employed in two and three space dimensions, respectively. The mesh is locally adapted to the solution according to the principle of $h$-adaptation. Hanging nodes, which occur due to the local refinement are maintained, i.e. no transition elements are introduced. Hence the adaptation remains local and the basic element type is preserved.

3.2 Adaptation

The grid adaptation is based on a multiscale analysis and data compression similar to techniques used for image compression. This is a new strategy independent of error indicators and error estimators. Here a strategy is followed that has been originally developed by A. Harten [43]. References [35], [36], [74], [75] provide the further details of employed multiscale technique for grid adaptation. Here a brief description is given. The concept for the grid adaptation strategy is outlined in three steps, namely,

- an array of cell averages is transferred into a new data format,
- thresholding techniques are applied to the new data format in order to reduce its complexity and
- a locally refined grid is determined by means of the compressed data format.
Step 1: In the first step, it is explained how to derive a new data format that will be useful to realize high compression rates. For this purpose, a sequence of nested grids \( \mathcal{G}_j := \{ \mathcal{V}_{j,k} \}_{k \in I_j}, j = 0, \ldots, L \), not necessarily structured, and related cell averages \( \mathbf{u}_j := \{ u_{j,k} \}_k \) of a scalar function \( u \) (see Fig. 3.1) is considered. Here \( j = 0 \) and \( j = L \) always denote the coarsest grid and the finest grid, respectively. The index set \( I_j \) represents the enumeration of the cells corresponding to the grid \( \mathcal{G}_j \). By means of this sequence, the averages \( \mathbf{u}_L \) on the finest level \( L \) is decomposed into a sequence of averages \( \mathbf{u}_j \) on the coarsest level and details \( \mathbf{d}_j, j = 0, \ldots, L - 1 \) (see Fig. 3.2). Here the cell averages \( \mathbf{u}_j \) can be viewed as a coarse grid approximation of the solution \( \mathbf{u}_L \), whereas the details \( \mathbf{d}_j \) describe the difference between the coarse grid approximation and the fine grid approximation. Of course, if the solution is smooth, then the difference will be small. For the construction of the details, the wavelet technique is employed.

![Figure 3.1: Sequence of nested grids](image1)

Step 2: In the previous step a new data format was introduced that is preferable to perform compression. The new format is composed of cell averages on a coarsest discretization level and arrays of details describing the difference information between the cell averages on two successive discretization levels. The detail coefficients become negligibly small in regions where the solution is sufficiently smooth. The index set of significant details \( \mathcal{D}_L := \{ (j,k) : \| u_{j,k} \| > \varepsilon \} \) is now introduced, that is related to all details that are larger than a level dependent threshold value \( \varepsilon_j = 2^{-j} \varepsilon \). The choice of the threshold parameter \( \varepsilon \) is discussed in [75].

Step 3: Next it remains to explain how to construct an adaptive grid by means of the index set of significant details. To this end, starting at the coarsest level, all cells are refined where a significant detail exists. If there is no significant detail, then the cell is not refined. Then the process proceeds with the next fine level and the same refinement strategy is applied to all existing cells of that level. This finally results in a locally refined grid with hanging nodes. It is to be noted that this strategy is only feasible if the index set \( \mathcal{D}_L \) of significant details corresponds to a graded tree, i.e. the levels of neighbouring cells differ at most by one.

![Figure 3.2: Multiscale Transformation](image2)
3.3 Finite volume discretization

The Navier-Stokes equations (eq. 2.9) can be written in integral form, which is the basis for a finite volume discretization. For an arbitrary control volume \( V \) with boundary \( \partial V \), eq. 2.9 becomes

\[
\left( \frac{\partial \mathbf{U}}{\partial t} \right)^{V} + \int_{\partial V} \left( \mathbf{F}_{i} - \mathbf{G}_{i} \right) \mathbf{n} \cdot dA = \int_{V} \mathbf{S} \, dV, \tag{3.2}
\]

where \( \mathbf{n} = (n_{x}, n_{y}) \) is the outward unit normal vector to the surface element \( dA \subset \partial V \). The state variables \( \mathbf{U} \), source term \( \mathbf{S} \), inviscid and viscous fluxes \( \mathbf{F}_{i}, \mathbf{G}_{i} \) and \( \mathbf{F}_{i}, \mathbf{G}_{i} \) respectively, are defined in chapter 2.

The discretization of the governing equations (eq. 3.2) is based on a cell centered finite volume scheme. Caused by the occurrence of hanging nodes, the grid is treated as a fully unstructured mesh with arbitrary polygonal/polyhedral control volumes in two and three space dimensions, respectively. The data structure of the flow solver is primarily based on the faces of the grid. A face based data structure has the advantage that there are no limitations on the number of faces, which can be assigned to a cell. Further, the evaluation of fluxes and their contribution to cells can be efficiently implemented by sweeps over the faces.

3.3.1 Numerical flux formulation

The discretization of the conservation equations for a small control volume results in a system of difference equations for the rate of change of the variables balanced by the normal fluxes over the cell interfaces. The variables used in the time derivatives usually are the volume-averaged values, whereas the fluxes need cell interface values.

3.3.1.1 Discretization of inviscid fluxes

The numerical formulation of the inviscid fluxes has a great influence on the properties of the solution method, since they contain the essential information of the wave transport [39]. A certain class of numerical schemes designed to stably discretize the fluxes arising from the hyperbolic equations is termed upwind schemes [46]. Today, upwind-biased schemes are the main trend of spatial discretization. Two types of upwind schemes exist. One family is based on a directional discretization of the flux terms according to the sign of the associated propagation speeds, the so-called Flux-Vector-Splitting (FVS) methods. Examples of FVS schemes are Steger and Warming [95], Van Leer [106] etc. The second family, Flux-Difference-Splitting (FDS), is based on an idea originally developed by Godunov [34]. This method solves for every mesh interval, the one-dimensional Riemann problem for discontinuous neighbouring states. This method results in a complex, time consuming solution procedure. Therefore, methods have been developed which give an approximate solution of the Riemann problem. Roe [87] and Osher [78], [93] FDS schemes are the most popular approximate Riemann solvers.
3.3 Finite volume discretization

FVS is based on scalar calculations while FDS is based on matrix calculations, so that FVS schemes are more robust and efficient than FDS schemes. It can be proved that FVS schemes like Steger and Warming [95] and Van Leer [106] are positively conservative under a CFL-like condition [37], [54], which is very desirable for simulating high-speed flows involving strong shocks and expansions. However, these schemes have accuracy problems in resolving shear layer regions due to excessive numerical dissipation, which occurs more seriously in hypersonic flow. Much effort has been spent on developing improved FVS-type schemes for high-speed flows, and they have shown reasonable enhancement in accuracy. FDS schemes, which exploit the solution of local Riemann problems usually provide more accurate solutions. The Roe [87] scheme is able to capture a shock and resolve the shear layer region very accurately. The Roe [87] scheme, however, has serious robustness problems such as the violation of entropy condition, failure of local linearization, and appearance of carbuncles [85]. Those defects become more serious in hypersonic flow than in subsonic or supersonic flow. Although an entropy fix may enhance the robustness, a large amount of entropy fix is usually required in hypersonic flow, which requires extra numerical dissipation. Determining the optimal amount of entropy fix without compromising accuracy is difficult and depends highly on the user’s experience. Some variants of Roe’s FDS such as the HLLE scheme [26] increase the robustness of Roe’s FDS at the expense of accuracy. Therefore the contemporary concern is shifted toward combining the accuracy of FDS and the robustness of FVS [54]. In an effort to design a numerical scheme to meet this concern, the AUSM [66] was proposed by Liou and Steffen. In AUSM, a cell interface advection Mach number is appropriately defined to determine upwind extrapolation for conserve quantities. As a result, AUSM is accurate enough to resolve a shear layer, and it is simple and robust. Thus AUSM possesses the merits suitable for the analysis of hypersonic flows. However, the characteristic of advection in AUSM may induce the oscillations of flow properties. Successively updated AUSM-type schemes such as AUSMD/V [110] and AUSM+ [65] did not overcome the problem perfectly [54]. AUSMD/V eliminates numerical oscillations or overshoes behind shock waves, though not completely, but may exhibit carbuncle phenomena. AUSM+ eliminates carbuncle phenomena but still shows numerical overshoes behind strong shock waves and oscillations near the region of small convection velocity or pressure gradient, such as near a wall or a stagnation point. A detailed comparison of various upwind methods have been made by van Keuk [104].

It is observed that no consensus of opinion has been reached concerning the ideal method for discretizing the inviscid fluxes. In the context of Riemann solvers, Quirk [85] suggested a strategy whereby the weaknesses of any one solver are overcome by combining it with one or more complementary solvers. This strategy can be applied to FVS scheme in the same way. The main advantages of this approach are that it does not degrade the resolution of the base solver; it is possible to control certain instabilities by changing the flavour of the dissipation mechanism rather than increasing the absolute level of dissipation.

In the context of the present work, upwind schemes like AUSM, AUSMD/V, AUSM+, Van-Leer FVS scheme have been extended for chemically reactive and vibrationally excited gas, and implemented into QUADFLOW. Since the present work mainly deals with hypersonic flows, where the
flow field is characterized by the presence of strong shocks, a hybrid strategy is adopted as suggested by Quirk [85]. To identify the shock locations, the pressure sensor as suggested by Quirk [85] is implemented. In this context, while working with AUSM, AUSMD/V and AUSM+ schemes, the Van-Leer FVS scheme is applied in the immediate vicinity of a strong shock wave. The Roe Riemann solver as extended for chemically reacting gas mixtures in thermochemical nonequilibrium, by Liu and Vinokur [67] and implemented and tested in the context of an ENO solver by Müller [73] has been additionally integrated in QUADFLOW.

### 3.3.1.2 Extension to higher order accuracy

In a cell centered finite volume procedure, flow variables are known in a cell-average sense. In order to evaluate the flux through a face, flow variables are required at both sides of the face. The FVS and FDS schemes are first order accurate, if the direct left and right values \( Q^L \) and \( Q^R \) represent the support of the reconstruction. The gradient of \( u \) is implemented. In this context, while working with AUSM, AUSMD/V and AUSM+ schemes, the reconstructed flow variable, \( u_i \) its mean value at the centroid \( c_i \) of \( \Omega_i \) and \( \phi_i \) denotes the limiter function. The reconstruction can be applied to the set of conservative variables, primitive variables or characteristic variables. In the present work, all of the computations employ reconstruction of primitive variables. The gradient \( \nabla u_i \) is obtained by employing the Green-Gauss theorem or a least squares method. In QUADFLOW, both methods have been implemented. In the context of the present work, Green-Gauss reconstruction method has been used.

As proposed by Barth and Jaspersen [3], the Green-Gauss theorem is applied to compute the average gradient of \( u \) over the surface of a bounding control volume

\[
\nabla u_i = \frac{1}{\Gamma_i} \int_{\Gamma_i} \mathbf{n} \, \mathbf{u} \, d\Gamma, \tag{3.4}\n\]

where \( \Gamma_i \) denotes a control volume, which is defined by the centroids of the neighbouring cells of \( \Omega_i \), which represent the support of the reconstruction.

In order to avoid oscillations in the vicinity of local extrema and discontinuities, limiter functions with TVD property are used. The limiter from Venkatakrishnan [108] has been employed which is defined as follows:

\[
\phi_{\text{lim}} = \begin{cases} 
\frac{w_{\text{lim}}^2 + 2w_{\text{lim}}^2 w_{\text{lim}} + \epsilon}{w_{\text{lim}}^2 + w_{\text{lim}}^2 w_{\text{lim}}^2 + 2w_{\text{lim}}^2 + \epsilon}, & \text{if } w_{\text{lim}}^2 \neq 0 \\
1, & \text{if } w_{\text{lim}}^2 = 0
\end{cases} \tag{3.5}
\]
3.4 Boundary conditions

with

\[
\begin{align*}
\varepsilon_g^+ &= \varepsilon_g^t - \varepsilon_t^t, \\
\varepsilon_g^- &= \begin{cases} 
\varepsilon_g^+ - \varepsilon_t^t, & \text{if } \varepsilon_g^+ > 0 \\
\varepsilon_g^- - \varepsilon_t^t, & \text{if } \varepsilon_g^- < 0
\end{cases}, \\
\varepsilon_{\max} &= \max(\varepsilon_{\kappa}, \varepsilon_{\tau}_j)_{j=1}^{N_s}, \\
\varepsilon_{\min} &= \min(\varepsilon_{\kappa}, \varepsilon_{\tau}_j)_{j=1}^{N_s},
\end{align*}
\]

where \( \varepsilon_g \) denotes the unlimited reconstructed value of \( \varepsilon \) at the Gauss quadrature point \( g \) and index \( j \) corresponds to the neighboring cells of cell \( i \). The coefficient \( \varepsilon \) is set depending on the applications. For typical hypersonic flow computations in the context of the present work, it varies between \( 10^{-4} \) and \( 10^{-6} \). Since condition (3.5) has to be fulfilled at each quadrature point of the faces, the final limiter associated with the control volume \( \Omega_k \) is taken as the corresponding minimum value \( \varepsilon_k = \min(\varepsilon_{\kappa}) \). Reference [11] describes the detailed implementation of this limiter in QUADFLOW.

3.3.1.3 Discretization of diffusive fluxes

Evaluation of diffusive fluxes require the determination of the gradients of the velocity vector, \( \nabla \mathbf{D} \), the temperature, \( \nabla T \) and the mass fraction of species, \( \nabla X_j \), at the cell interfaces. Some of the methods of discretization of the diffusive fluxes on unstructured grids are described in references [19], [20], [44], [52], [112]. Reference [11] describes integration of different methods in the QUADFLOW code, in the context of ideal gas flows. The methods can be used in their basic form to compute the gradient of the flow variables corresponding to real gas flows. In the context of the present study, the gradient of a flow variable is computed as follows [11]:

\[
\nabla \varepsilon_{\text{face}} = -\left( \nabla \varepsilon_{\text{face}} \frac{L_{LR}}{|U_{LR}|} - \frac{U_{LR} - U_{LT}}{|U_{LR}|} \right),
\]

(3.6)

where \( \nabla \varepsilon_{\text{face}} \) is the averaged gradient, \( \nabla \varepsilon_{\text{face}} = \frac{1}{2}(\nabla_{LR} + \nabla_{LT}) \). \( \nabla_{LR}, \nabla_{LT} \) are the gradients in the left and right cell centres of the face from inviscid reconstruction. \( L_{LR} = x_R - x_L \) is the direction connecting the centroids of left and right cells of the face.

3.4 Boundary conditions

The boundary conditions play an important role in numerical simulation of the flow fields. In most of the physical situations, they can be divided in in- and outflow conditions, and wall conditions. The cell–centered finite volume approach permits an attractive implementation of the boundary conditions. In this method, the unknowns are located at the cell centroid and not on the boundary; thus a direct modification of these values to apply the boundary conditions is not very well suited. On the
contrary, the boundary conditions may be enforced in the formulation of the flux at the boundary edges. This corresponds to a weak formulation of the boundary conditions but is found very efficient in practice and has the advantage that boundary cells are treated in the same way as interior cells \[22\].

### 3.4.1 Supersonic inflow condition

In case of supersonic inflow, there are no outgoing characteristics from the computational domain to the boundary point. Therefore all flow quantities at the boundary are prescribed.

### 3.4.2 Supersonic outflow condition

At supersonic outflow, all characteristics from a boundary point leave the computational domain. Therefore, a linear extrapolation is made from the interior cells to the boundaries.

### 3.4.3 Wall boundary

In case of inviscid computations, the flow tangency condition, \( \mathbf{v} \cdot \mathbf{n} = 0 \), is enforced at the solid wall. This condition yields the flux formula at the wall as

\[
\mathbf{F}_{nw} \cdot \mathbf{n} = (0, \rho v, \mathbf{n}, 0),
\]

where the static pressure at the wall is extrapolated from the interior domain.

For viscous flow, a no-slip boundary condition is applied, where the flow velocity, both normal and tangential to the surface is zero. Also at the wall, the normal pressure gradient is assumed to be zero, i.e., \( \frac{\partial p}{\partial n} = 0 \), where \( n \) corresponds to the normal direction. A thermal condition has also to be enforced.

For isothermal wall, the condition \( T = T_{wall} \) is imposed. An additional boundary condition must be supplied for the chemically reacting flows with mass diffusion. The solid wall can be treated as fully catalytic, where the mass fractions at the wall would be at the equilibrium value corresponding to the prescribed wall temperature, \( T_{wall} \). For a noncatalytic wall, there is no chemical reaction at the wall, and therefore, a zero mass fraction gradient is imposed, i.e., \( \frac{\partial Y}{\partial n} = 0 \). In the present study, the wall is treated as isothermal and noncatalytic. The boundary conditions are implemented through the modification of the fluxes through the wall.

### 3.4.4 Plane of symmetry

The boundary conditions at a plane of symmetry is same as that of slip boundary condition. The flow tangency condition, \( \mathbf{v} \cdot \mathbf{n} = 0 \), is enforced at the symmetric wall, which results in the flux formula as given in eq. 3.7.
3.5 Time-integration

The integration of eq. 3.2 in an arbitrary control volume, \( V \), gives

\[
\frac{d\mathbf{U}}{dt} V + \sum_{f} F_{i,f} - \sum_{f} F_{i,f} = S \cdot V = \sum_{f} \frac{dU_i}{dt} V = -\mathbf{R}(\mathbf{U}) + S \cdot V ,
\]

(3.8)

where \( \mathbf{U} \) is the cell averaged conserved variable, and \( F_{i,f}, F_{i,f} \) are the numerical inviscid and viscous fluxes, respectively at face \( f \).

The above equation can be advanced in time either in a fully coupled way, where the thermochemical source term \( S \) is advanced in time simultaneously with \( \mathbf{U} \) or, in an operator-splitting way [96], [101], [105]. The splitting of the equations is done as follows:

\[
\frac{d\mathbf{U}}{dt} V + \mathbf{R}(\mathbf{U}) = 0 ,
\]

(3.9)

\[
\frac{d\mathbf{U}}{dt} = S
\]

(3.10)

The physical meaning of this splitting procedure is that during the first half-step of time integration, an inert fluid is allowed to convect and diffuse, whereas during the second half-step a fluid at rest is allowed to react thermochemically. The resulting system of equations is solved by an explicit multistage Runge-Kutta scheme. Convergence to steady state is accelerated by local time stepping. The implementation of the explicit time integration procedure in QUADFLOW is described in Ref. [11].

For the computation of flows in thermochemical equilibrium, instead of solving eq. 3.10, a system of nonlinear algebraic equations has to be solved, to get the equilibrium composition of the air. Reference [2] describes the details about the system of equations, to be solved for a thermochemical equilibrium gas model. The method of solution for the system of algebraic equations is more complicated than ordinary differential equations. In the context of the present work, the curve fit of Prabhu et al. [84] is used, to get the equilibrium composition of air. The equilibrium thermodynamic properties is determined using the curve fit of Srinivasan et al. [94].

3.6 Two-dimensional axisymmetric Euler equations

Although three-dimensional CFD calculations are state of the art, axisymmetric flow solvers are indispensable tools, for cases which allow their applicability. The governing equation of motion for the two-dimensional axisymmetric inviscid flow [47], [118] is expressed as

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial (\mathbf{F}_{\text{inv}})}{\partial x} + \frac{\partial (\mathbf{G}_{\text{inv}})}{\partial y} + \mathbf{H} = \mathbf{S},
\]

(3.11)

where the vectors \( \mathbf{U}, \mathbf{F}_{\text{inv}}, \mathbf{G}_{\text{inv}} \) and \( \mathbf{S} \) are same as defined in eq. 2.9. The source term \( \mathbf{H} \) arising out as a result of axisymmetric flow field, is given as

\[
\mathbf{H} = \frac{1}{\gamma} \left[ \rho \mathbf{v}, \rho u \mathbf{v}, \rho v \mathbf{v}, \rho, \rho u \mathbf{v}^2, \rho v \mathbf{v}^2, \rho \mathbf{v} \mathbf{v} \cdot \mathbf{v} \right] \right]^T
\]

(3.12)
The numerical treatment of the geometrical source term $H$ is similar to that of the thermochemical source term $S$.

### 3.7 One-dimensional Euler equations for steady flow

The Euler equations for a one-dimensional, steady flow in thermochemical nonequilibrium, can be expressed as

\[
\frac{d\lambda_{\alpha}}{dx} = \frac{1}{\Psi} \frac{\partial \psi}{\partial \lambda_{\alpha}}, \quad \lambda_{\alpha} = 1, N - 1 \tag{3.13}
\]

\[
\frac{d\epsilon^{(j)}}{dx} = \frac{1}{\Psi \rho} \frac{\partial \epsilon^{(j)}}{\partial \epsilon^{(j)}}, \quad j = 2, I \tag{3.14}
\]

\[
\frac{dp}{dx} = \frac{\alpha^2}{\gamma u^2 - a^2} \cdot \Phi \cdot p \tag{3.15}
\]

\[
\frac{d\rho}{dx} = \frac{\alpha^2}{\gamma u^2} \left( \frac{u^2 - a^2}{u^2} \right) \cdot \Phi \cdot \rho \tag{3.16}
\]

\[
\frac{du}{dx} = -\frac{\alpha^2}{\gamma u^2} \left( \frac{u^2 - a^2}{u^2} \right) \cdot \Phi \cdot u \tag{3.17}
\]

The term $\Phi$ describes the effect of the relaxation processes on the density and the pressure. It is expressed as

\[
\Phi = (\gamma - 1) \frac{\rho}{p} \left\{ \sum_{j=2}^{I} \frac{d\epsilon^{(j)}}{dx} + \sum_{\alpha=1}^{N} \left[ \alpha^{(0)} \epsilon^{(0)} + \alpha^{(1)} \epsilon^{(1)} - \frac{R_{T(1)}}{\gamma - 1} \frac{d\lambda_{\alpha}}{dx} \right] \right\}, \tag{3.18}
\]

where $I$ denotes the total number of temperatures to be considered.

The above system of equations represent a system of nonlinear, ordinary differential equations, which can be solved as initial value problem. In the present study, this system of equations was used to compute the one-dimensional, steady flow behind a normal shock. The flow conditions just behind the normal shock were taken as the initial values. The DLSODE solver of ODEPACK package [45], [86] was used to solve the equations.
Chapter 4

Relaxation behind normal shocks

The condition behind a stationary normal shock wave can be determined by means of the classical equations for the calorically perfect gas as long as the free stream Mach number is at the lower spectrum of the hypersonic flow regime. Increasing the free stream Mach number from a supersonic value, the temperature behind the normal shock waves, at certain Mach number, becomes so high that the internal energy modes of the molecules are excited and chemical reactions take place. The flow field then deviates considerably from the calorically perfect gas model.

In such a situation, the flow process can be modelled as shown in Fig. 4.1. The free stream condition in a real hypersonic flight in the atmosphere is given by \( \rho_\infty, \beta_\infty \) and \( T_\infty \) in thermal and chemical equilibrium. If the free stream is produced in a laboratory through the expansion of the flow in the nozzle, then it may be in thermochemical nonequilibrium. In such case, to completely describe the free stream, additionally, among others, the molar vibrational energy \( (e_v)_\infty \) and mass composition of the free stream \( (X_j)_\infty \) is required. Starting from this condition, through a shock zone of a few mean free path, the gas is brought to a condition 1, where translation, rotation and electronic energy is in equilibrium and vibration energy and chemical composition in the shock zone is frozen. Since the thermal and chemical equilibrium is disturbed at condition 1, the nonequilibrium flow develops behind it, which finally approaches an equilibrium value at condition 2. This zone behind the normal shock where a nonequilibrium flow relaxes towards equilibrium condition is called the relaxation zone. This relaxing flow field is completely described by the governing equations as derived in section 3.7.

The rate at which the relaxation processes occur behind strong shock waves has an important effect on the flow field around high-speed missiles and re-entering vehicles. For a re-entry speed of around 7000 m/s, the translational temperature immediately behind the bow shock may reach around 24000 K and the rate at which this temperature declines to equilibrium values of around 6000 K depends on the rates of the many complex chemical reactions and energy exchanges which occur. The study of relaxation processes behind a normal shock wave is an excellent numerical test case to investigate the influence of different physicochemical modelling on the overall flow field. In this chapter, the stationary, inviscid one dimensional flow of a five component air in thermal and chemical
nonequilibrium behind a normal shock is investigated. The essential features of the relaxation process are discussed through the numerically calculated distribution of the flow variables for different free stream velocities. Finally using computational result, the binary scaling law is verified.

The free stream conditions and conditions directly behind normal shock for test cases being investigated are given in Table 4.1. These test cases are taken from [55]. These test conditions are representative of hypersonic flow regimes from the low enthalpy range (case C1) to the high enthalpy range (case C3). Case C2 is a bridge between C1 and C3. The free stream is assumed to be in thermochemical equilibrium. In the computations, different sets of chemical rate constants and thermal models are used and their influence on the flow field are discussed. Figure 4.2 shows the distribution of pressure, velocity and density plotted against the distance from the normal shock which is located at \( x = 0 \). These flow variables have been normalised with the corresponding values existing just behind the shock. As shown in the Fig. 4.2, the relaxation process proceeds with nearly constant pressure. This

<table>
<thead>
<tr>
<th>Test Case</th>
<th>( V_\infty [\text{m/s}] )</th>
<th>( p_\infty [\text{Pa}] )</th>
<th>( T_\infty [\text{K}] )</th>
<th>( \rho_1 [\text{kg/m}^3] )</th>
<th>( T_1 [\text{K}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>4000</td>
<td>100</td>
<td>300</td>
<td>678</td>
<td>15420</td>
</tr>
<tr>
<td>C2</td>
<td>6000</td>
<td>100</td>
<td>300</td>
<td>945</td>
<td>35070</td>
</tr>
<tr>
<td>C3</td>
<td>9000</td>
<td>100</td>
<td>300</td>
<td>1234</td>
<td>80690</td>
</tr>
<tr>
<td>C4</td>
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<td>13835</td>
<td>2701</td>
<td>1232.9</td>
<td>387800</td>
</tr>
<tr>
<td>C4*</td>
<td>6165</td>
<td>13835</td>
<td>2701</td>
<td>1161.3</td>
<td>477560</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Test Case</th>
<th>( X_N )</th>
<th>( X_{O_2} )</th>
<th>( X_O )</th>
<th>( X_{O_2} )</th>
<th>( X_{NO} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C4</td>
<td>0.000</td>
<td>0.7753</td>
<td>0.196</td>
<td>0.027</td>
<td>0.022</td>
</tr>
<tr>
<td>C4*</td>
<td>0.000</td>
<td>0.7653</td>
<td>0.255</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

Table 4.1: Free-stream conditions
fact is generally valid for stationary, one dimensional flow with constant cross-sectional area. On the other hand, the profiles of density and velocity show large changes. Figures 4.3 to 4.13 show the plots of mass fraction of molecular components and temperatures for the test cases C1 to C3. Unless otherwise mentioned in the figure, all the results are obtained using the nonpreferential dissociation model. In the plots, the temperatures are normalised with the value of translational temperature directly behind the normal shock. With these plots, some essential features of relaxation processes are described. From these plots, among other things, the significant influence of kinetic energy of the free stream on the length of relaxation zone is to be seen (compare especially Figs. 4.3 and 4.4). The influence of free stream kinetic energy on the degree of dissociation of molecular components at equilibrium condition is also clear from these plots.

For the test case C1, the vibrational relaxation time of $O_2$ and $NO$ is smaller than the characteristic time of chemical reactions. Therefore the vibration energy transfer through reactive collisions is of
not much significance. Under the condition of test cases C2 and C3, the chemical reactions run widely under vibrational nonequilibrium, since chemical reactions and vibrational relaxation times are of the same order. For test case C2 (Fig. 4.4), it is observed that the equilibrium condition \( T_{O_2}^{(0)} = T^{(v)} \) is arrived at the position behind the normal shock, where the mass fraction of \( O_2 \) approaches a steady value. This is also observed in other figures. The mass fraction of \( N_2 \) approaches towards steady value when the complete thermodynamic equilibrium is achieved. These phenomena become more pronounced with increasing dissociation rate, as is evident from Fig. 4.5. The reaction rate constants used for the computation corresponding to Fig. 4.5 is from Park (90), which is greater than otherwise used rate constants of Dunn and Kang, Gupta and Park (87), as shown in Figs. 4.4 to 4.5. Due to high dissociation rates, one temporary dissociation related freezing of vibration temperatures of \( O_2 \) and \( N_2 \) is observed just behind the shock. Out of various chemical models used here, the Gupta model is found to be slowest and thus as is evident from Fig. 4.6, the approach to equilibrium is delayed. The influence of different chemical models on the relaxation process is clearly seen. Even though the relaxation curves for \( N_2 \), \( O_2 \) and \( NO \) differ in the Figs. 4.4- 4.5, the final equilibrium condition is same.

In Ref. [55], Klomfaß observed that the vibrational relaxation of nitric oxides depends considerably on the concentration of this component in the free stream. The NO molecules which are produced as a consequence of Zeldovich reactions behind the normal shock, possess according to the Random Recombination model an infinitesimally high vibrational temperature. Thus immediately behind the normal shock, two different Boltzmann distributions exist with \( T_{NO}^{(0)} \to \infty \) and \( T_{NO}^{(v)} = T_{NO}^{(0)} \). Under the assumption of unrestricted equilibrium internal to inner energy modes, immediately behind the normal shock, a new Boltzmann distribution is reached. The resulting vibration temperature which depends on the total vibrational energy of NO, goes to infinitesimally high value, with vanishing NO fraction in the free stream. Therefore in the computation always little amount of \( NO \) is introduced. Following the observation of Klomfaß, in the present work the mass fraction of \( NO \)
in the free stream is set to be $1 \cdot 10^{-1}$. However, as it will be observed in Fig. 4.14, the vibrational temperature of NO does not rise very fast with the Millikan and White model, as it is the case for the Klomfass model. Except the VT model, all other parameters are same for both the computations. Therefore, it is evident that the higher VT rates of NO in case of the Klomfass model is the main cause for the sudden rise of vibrational temperature of NO.

The meaning of VV-transfer in the relaxation process is made obvious by comparing the Figs. 4.8 and 4.10. In Fig. 4.10, the VV-transfer of all molecular components are neglected. As a consequence of it the vibration temperature of NO takes a very high peak value, during which the maximum occurring vibrational temperature of N2 diminishes. The effect of VV-transfer on the $O_2$ relaxation is comparatively small, since on one hand vibrational energy is given to slow relaxing $N_2$ and on the other hand it gains vibrational energy from the fast relaxing NO. In Fig. 4.10, the observed overshoot of $T_{\text{NO}}$ over the translational temperature is a consequence of the high energy associated with the NO molecules which are produced as a result of the Zeldovich reaction. This behaviour is also observed with the test cases C1 and C2.

In the results presented so far, the free stream was assumed to be in thermochemical equilibrium. The flow in the test section of a shock tunnel is found to be in nonequilibrium condition. Considering this practical situation, one test case is considered to investigate the influence of a nonequilibrium free stream on the relaxation process. Figure 4.11 shows the distribution of the normalised temperature and the mass fractions, which was calculated for the test case C4. The free stream exhibits a higher fraction of atomic oxygen in thermal equilibrium. For comparison purpose, a test case is selected which has free stream in thermochemical equilibrium and has the same value of density, pressure and total enthalpy. The free stream condition for this test case is marked as C4* in Table 4.1. The distribution of normalised temperature and the mass fractions for this test case is shown in Fig. 4.12. In both cases, identical equilibrium condition is arrived after the relaxation processes. The distinguishable difference in the figures with regard to equilibrium condition, is due to the different temperatures
behind the shock, which are used as references. The comparison of the figures show very little difference in the relaxation of vibrational temperatures of $N_2$ and $O_2$.

The comparison of Figs. 4.8 and 4.9 shows that in case of the preferential dissociation model, the approach to equilibrium condition is delayed. In case of the preferential dissociation model, the chemical reaction rate is quite slower than that for the nonpreferential model which slows down the fall of translational mode of energy and thus translational temperature of the flow field. At the same time, molecules at high excited energy states have preference over lower energy states molecules to dissociate. This process works against the equilibration of vibrational temperature to translation temperature. Thus these two processes together delay the approach to equilibrium. The slowing of chemical reaction rate due to preferential dissociation model is suitable for numerical solvers as the system of equations become significantly less stiff. In the present computation, the solver was more than 30 times faster in case of the preferential model than that for the nonpreferential model.
In the next results, the concept of binary scaling is verified. The concept of the binary scaling law is as follows: For two different flows, where the flow field is dominated by the two-body dissociation reactions rather than the three-body recombination reactions and having same \( T_{sc} \) and \( V_{sc} \) but different values of \( \rho_{sc} \) and \( L \) (reference length), the results will be the same if the product \( \rho_{sc} L \) remains the same between the two flows. To verify this law, the plots of the temperatures and the mass fractions for two free stream conditions are put one above another as shown in Fig. 4.13. The case (1) corresponds to the test case C2 and the case (2) corresponds to a test case where free stream density and the pressure in test case C2 is increased by a factor 100. Following the concept of the binary scaling law, the distance from the normal shock is normalised with the reference lengths as given below:

\[
\frac{L_{ref}^{(1)}}{L_{ref}^{(2)}} = \frac{\rho_{sc}^{(2)}}{\rho_{sc}^{(1)}}
\]  

(4.1)

In the figure, the plot in case (1) and case (2) are represented by lines and symbols respectively. As is evident from the figure, the plots are identical in the relaxation zone close to the normal shock, where the flow field is dominated by dissociation reactions. At the more downstream of the relaxation zone some difference in the plot is seen. It happens due to increased significance of three-body recombination reactions. The final equilibrium condition depends on the free stream density and velocity. The equilibrium condition which the flow finally arrives at in this case is different because of difference in free stream densities. Therefore the flow similarity at the later stage of the relaxation zone is not achieved. The concept of binary scaling is therefore suitable only for such a flow field where the dimension of the test model is noticeably smaller than the length of the relaxation zone.

In Ref. [81], Park points out the benefit of including the nonequilibrium vibrational energy as an additional dependent variable: the computation becomes insensitive to the numerical errors, and the chemical reactions become less stiff behind a shock wave. In an one-temperature model, the temperature at the first node point behind a shock wave is very high, and so the chemical reaction rates become very large. A small numerical error in the post shock conditions results in a large error in the rate of dissociation at that point. In a two-temperature model, the vibrational temperature is very low behind the shock, and so chemical reaction rates are nearly zero there because in this case the average temperature is very low. Chemical reaction rates become large only after a few node points. Thus in the study of thermal nonequilibrium, a question arises whether it is worthwhile to increase the number of vibrational temperatures. An attempt is made to answer this question using 1D results for test case C2, as shown in Figs. 4.14-4.16. In all these three results, the thermochemical models remain same except for the vibration-translation energy exchange. Figure 4.14 shows the comparison of Klomfaß and Millikan and White vibration-translation model. Though the relaxation length is nearly the same for both models, the approach to equilibrium is different. The VT rates of \( N(O) \) in case of the Klomfaß model is higher than that of the Millikan and White. This is the reason why the vibrational temperature curve of \( N(O) \) with the Klomfaß model lies higher than that of the Millikan and White model. Figure 4.15 shows a comparison of a four temperature and two temperature model. The vibration-translation model of Klomfaß is used for this case. It is to be noted that the relaxation
length in both temperature models do not differ significantly. The translation temperature curve differs before the approach of thermal equilibrium. On the other hand, the comparison of the two and four temperature models with Millikan and White VT model, as shown in Fig. 4.16 show negligible difference with regard to translation temperature. In conclusion, different modelling of the energy exchange processes yields a different behaviour of the flow field. Thus considering the uncertainties associated with the modelling of different energy exchange processes, it may not be worthwhile to introduce more and more temperatures in CFD calculation. The introduction of more and more temperatures even brings back the problem of numerical stiffness.
Figure 4.10: Nondimensional profiles of $X_e$, $T^{(e)}$, Park (90) rate constants, no VV-transfer, condition C3

Figure 4.11: Free stream in nonequilibrium, Park (90) rate constants, preferential dissociation, condition C4

Figure 4.12: Free stream in equilibrium, Park (90) rate constants, preferential dissociation, condition C4*
Figure 4.13: Binary scaling law, Park (90) rate constants, condition C2

Figure 4.14: Comparison of VT models (solid lines with symbols: Klomfaß, broken lines: Millikan and White), Park (90) rate constants, condition C2

Figure 4.15: Comparison of vibration temperature models (solid lines with symbols: 4 temperature model, broken lines: 2 temperature model), Park (90) rate constants, Klomfaß VT model, condition C2
Figure 4.16: Comparison of vibration temperature models (solid lines with symbols: 4 temperature model, broken lines: 2 temperature model), Park (90) rate constants, Millikan and White VT model, condition C2
Chapter 5

Computation of two dimensional flows

5.1 Inviscid nonreactive flow over a double ellipse

The inviscid flow over the double ellipse is a well known test case proposed in the workshop of Antibes [23]. The double ellipse is placed in a hypersonic flow with a Mach Number equal to 8.15 and incidence angle of 30 degrees. The initial mesh of 4640 quadrilaterals is adapted seven times. The initial and final mesh is shown in Figs. 5.1 and 5.2. The iso lines pattern for $C_p$ and Mach number is presented in Figs. 5.3 and 5.4, respectively for the last adapted mesh computation. For this test case, the Van Leer’s flux vector splitting method is employed. Explicit Runge-Kutta 4 stage method is used for time integration. Figures 5.5 and 5.6 show the distributions of the pressure coefficient and the Mach number along the windward and leeward sides. The results are compared with those obtained by Gustafsson et al. and Khalfallah et al., published in the workshop proceedings [23]. The pressure coefficient and the Mach number distribution agree quite good with the results of the later authors. Iso-$C_p$ and density lines clearly show the robustness of the code in resolving the bow and canopy shock. This is also evident from the wall distribution of the $C_p$ and Mach number. The resolution of the bow shock and canopy shock is found to be far better than other investigators of the proceedings [23]. A detached normal shock is found at the canopy corner which becomes visible in a zoom of e.g. Figs. 5.3 and 5.4. This behaviour can also be predicted by the use of the oblique shock relations. For a deflection of 41.5 degrees in the canopy corner, these relations state that the Mach number at the nose upstream of the canopy should be at least about 5.4 in order to have an attached shock which is not the case for the present test case. The bending of the iso-Mach lines towards the wall illustrates the presence of an entropy layer. This entropy layer is created at the stagnation region in front of the nose and is then convected along the wall boundaries of the double ellipse.

5.2 Inviscid air flow over a circular cylinder

The hypersonic inviscid air flow over a circular cylinder was investigated, with the free stream conditions as given in Table 5.1. The cylinder has a diameter of 0.0406 m. The computation was made
5.2 Inviscid air flow over a circular cylinder

Figure 5.1: Double ellipse: Initial mesh
Figure 5.2: Double ellipse: Final mesh

Figure 5.3: Double ellipse: Iso-$C_p$ lines
Figure 5.4: Double ellipse: Iso-Mach lines
considering calorically perfect, chemical nonequilibrium and thermochemical equilibrium gas models. The aim of this study is to see the real gas effects on the shock stand-off distance. Figure 5.7 shows the iso-density plot for the three different flows. The comparison of density and temperature distribution along the stagnation line is shown in Figs. 5.8 and 5.9, respectively. The shock stand-off distance is smallest in the case of calorically perfect gas and the chemical nonequilibrium flow shock stand-off distance lies between calorically perfect gas and thermochemical equilibrium flow. In case of calorically perfect gas, the directed kinetic energy of the flow ahead of the shock is mostly converted to translational and rotational molecular energy behind the shock. On the other hand, for a gas in thermal equilibrium and/or chemically reacting gas, the directed kinetic energy of the flow, when converted across the shock wave, is shared across all molecular modes of energy, and/or goes into the dissociation energy of the products of the chemical reactions. Hence, the temperature which is a measure of translational energy only, is less for such a case. In contrast, the pressure ratio is affected only by a small amount since pressure is a "mechanically" oriented variable and it is governed mainly by the fluid mechanics of the flow and not so much by the thermodynamics. The combined effect of pressure and temperature yields the density ratio across the shock which will be more pronounced in case of a gas with internal energy excitation and/or chemically reacting gas. The shock stand-off distance, which depends on the density ratio across the shock, therefore in this case will be less as for nonreacting gas [2], [60]. The results shown confirm the above observations. The comparison of wall pressure coefficient and wall temperature distribution is shown in Figs. 5.10 and 5.11, respectively.
5.2 Inviscid air flow over a circular cylinder

Figure 5.7: Iso-Density plots (left: calorically perfect, center: chemical nonequilibrium, right: thermochemical equilibrium)

The significant influence of real gas effects on the temperature distribution over the cylinder surface is clearly to be seen. There is very little influence of real gas on the $C_p$ distribution over the wall. The accuracy of the present computation is again shown by comparing the shock stand-off distance and post normal shock temperature for the calorically perfect gas. The post normal shock temperature in case of a calorically perfect gas is given by [120]:

$$T_S = T_{\infty} \left( 1 + \frac{3(\gamma - 1)M^2}{2} \right)$$  \hspace{1cm} (5.1)

The analytical post shock temperature as calculated using eq. 5.1 is 6519 K and the computed value is 6614 K. Thus an excellent agreement between analytical and computational result has been achieved. In Ref. [2], the approach to determine the property variation across a normal shock, considering thermodynamic equilibrium is explained. The post normal shock temperature for the present test case in thermodynamic equilibrium, as determined from this approach is 3342 K, which is in quite good agreement with the computed value of 3430 K.

The empirical correlation of Billig [2], [4] for the shock stand-off distance in case of a cylinder, which is valid for calorically perfect gas is given as:

$$\frac{\Delta}{R} = \frac{2086 \gamma}{M^2} \left[ \frac{\gamma T}{M^2} \right]$$  \hspace{1cm} (5.2)

The agreement regarding the shock stand-off distance between the present computation and as calculated using eq. 5.2 is quite good, as shown in Fig. 5.9.
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Figure 5.8: Density distribution along the stagnation line

Figure 5.9: Temperature distribution along the stagnation line

Figure 5.10: $C_p$ distribution on the cylinder surface

Figure 5.11: Temperature distribution on the cylinder surface
5.3 Nitrogen flow over a circular cylinder

The study of one dimensional flow, as discussed in chapter 4, provided an overview of various aspects of different thermochemical modelling on relaxation processes behind a normal shock. In this section, results of a similar study considering two dimensional nitrogen flow over a circular cylinder are presented. The free stream conditions taken from one of the experiment of Hornung [50] are given in Table 5.2. The cylinder has a radius of 0.0127 m. It is assumed that the vibrational energy of the free-stream is in equilibrium with other modes of energy and thus $T_{V_2}^{(0)} = 1833$ K. The numerical simulations were mainly carried out for inviscid flow, since the purpose of this study is to highlight the influence of different thermochemical models on the overall flow field. However, additionally a viscous flow computation for the same test case was also performed (see Figs. 5.45-5.47).

An initial mesh of 6000 cells is adapted three times. The final mesh has 30126 cells. The initial and final meshes are shown in Fig. 5.12. Figure 5.13 shows the zoomed view of the final mesh, depicting the grid adaptation near the bow shock and stagnation region. Figure 5.14 shows the iso-density plot on the first and last mesh, respectively. The computations were made with Park(85) chemical kinetic model [79]. The vibration-dissociation coupling of Treanor and Marrone [69], [102] with nonpreferential dissociation was considered. For vibration relaxation time required in vibrational-translation relaxation model, the model of Klomfaß [55] was used. The distributions of pressure, density and atomic nitrogen mass fraction along the stagnation line for the first and last mesh are compared in Fig. 5.15. For the coarse grid, the smearness of the bow shock is clearly seen from this comparison. It is quite evident that the proper resolution of different features of the flow field requires a proper grid adaptation, which is effectively done in this case by the multiscale grid adaptation algorithm.

Iso plots of density, atomic nitrogen mass fraction, temperatures and corresponding distributions along the stagnation line on the final mesh are shown in Figs. 5.16-5.19. For this computation, the chemical kinetic model of Park(90) [81] was used. The vibration-dissociation coupling of Treanor and Marrone [69], [102] with nonpreferential dissociation was considered. For the vibration relaxation time required in the vibrational-translation relaxation model, Klomfaß [55] model was used. The resolution of the flow field is clearly seen. The pressure at the stagnation point is increased nearly by 50 times to the free stream value. Most of the pressure increase takes place due to the bow shock but isentropic compression between the bow shock and the stagnation point moderately increases the pressure. The translational temperature just behind the shock reaches a value of around 15000 K, whereas the vibration temperature remains at its free stream value, since excitation of vibrational mode needs a significant number of collisions compared to fewer collisions required for the translational...
Figure 5.12: Initial and final mesh

Figure 5.13: Zoomed view of the final mesh

Figure 5.14: Iso-density lines on initial and final mesh

Figure 5.15: Distribution of pressure, density and atomic nitrogen mass fraction along the stagnation line
mode. Behind the bow shock, the high enough translation temperature initiates chemical reactions. The translation temperature starts falling at one hand due to the molecular nitrogen dissociation, and on the other hand due to the translation-vibration relaxation process. The vibrational energy at one hand increases due to translation-vibrational energy exchange and on the other hand, it loses to dissociation due to vibration-dissociation coupling. Overall the vibration energy pool increases before finally approaching the equilibrium value at the stagnation point. It is clear from the plots that a significant thermal and chemical nonequilibrium takes place between the bow shock and the stagnation point. The dissociation of molecular nitrogen takes place in vibrational nonequilibrium. The rise in density in this region is as much as caused by bow shock compression. In the expansion region of the cylinder, the chemical reaction is frozen, as is shown by parallel contour lines of atomic nitrogen mass fraction. On the other hand, iso contour lines of temperatures show a gradient in this region. Figures 5.20 and 5.21 show the comparison of three chemical kinetic models, Park(85) [79], Park(90) [81] and Gupta [38]. For all the three cases, the vibration-dissociation coupling of Treanor and Marrone [69], [102] with nonpreferential dissociation was considered. For the vibration relaxation time required in vibrational-translation relaxation model, the Klomfaß [55] model was used. The shock stand-off distance is largest with Park(85) model and smallest in case of Gupta’s model. This is consistent with the fact that, the rate constants for $N_2$ dissociation for Park(85) model is smaller than Gupta. The result for the Park(90) model lies in between Park(85) and Gupta. The larger reaction rates result in fast dissociation of molecular nitrogen as is evident in plots of atomic nitrogen in Fig. 5.21. The dissociation takes energy from the flow field. Thus the fast dissociation of molecular nitrogen will result in a rapid drop in the translational temperature of the flow. Since the pressure is nearly constant between the shock and stagnation point, the fast drop of translational temperature results in a fast rise of density and hence in turn smaller shock stand-off distance. All the three models show nearly same temperatures along the wall away from the stagnation point, as shown in Fig. 5.22. At
the stagnation point, again the difference is observed due to different reaction rates. Park(85) shows a higher temperature at the stagnation point. All the chemical models show the same distribution along the wall, as shown in Fig. 5.23. This is consistent with the fact that the pressure is mainly driven by fluid mechanics of the flow and is not affected by chemistry. Figures 5.24-5.27 show the comparison of experimental and computational interferograms of the flow field for different chemical models. The basics of the interferogram technique is given in Appendix C. The agreement regarding the shock stand-off distance is quite satisfying but the differences in the flow field are clearly seen. Thus it is inferred that the shock stand-off distance is not a sufficient parameter to validate the phy-
5.3 Nitrogen flow over a circular cylinder

It is observed from the figures that Park(90) rate sets together with the VT and VV transfer rates of Klomfaß produces the flow field which is in quite good agreement with the experimentally obtained flow field. The differences with Park(85) and Gupta model in the expansion area as well as near the stagnation point is clearly seen. The experimentally obtained interferogram shows an initial compression of the gas directly behind the oblique shock in the upper regions of Fig. 5.24. It appears as a thin brighter fringe. The computational interferogram in this region shows the expansion of the flow. The observed compression can be as a consequence of the finite length of the cylinder which introduces a curvature to the shock front.

For the temperature range of the present test case, the vibrational relaxation time becomes comparable with that for dissociation. Thus the extent of vibrational nonequilibrium and the variation of the relative probability of dissociation from the excited levels considerably determine the overall rate of molecular dissociation. In case of the nonpreferential dissociation model, dissociation occurs with equal probability from any vibrational level in any collision that has sufficient translational energy to effect the dissociation. For the Treanor and Marrone model, nonpreferential dissociation corresponds to \(U = \infty\). In case of the preferential model, the dissociation probability is higher for higher vibrational levels. The molecules have to first ladder climb to come to a higher excited level before dissociation takes place. Thus a lag in vibrational excitation has the effect of inhibiting the dissociation process, because of the lack of highly excited (and thus easily dissociable) molecules. Thus the rate of dissociation is smaller in case of preferential dissociation model compared to nonpreferential model. The slower dissociation corresponds to larger shock stand-off distance and lower density rise as is evident in Figs. 5.29 and 5.30. The comparison of interferograms as shown in Fig. 5.28 clearly shows the differences in the flow field. From the numerical point of view, the fast dissociation rate associated with the nonpreferential model makes the system of equations to be solved more stiffer. At the stagnation point, translational and vibrational temperature of \(N_2\) are closer
Figure 5.24: Experimental interferogram of Hornung [50]

Figure 5.25: Comparison of interferograms (top: computed interferogram (Park85 model), bottom: experimental interferogram)

Figure 5.26: Comparison of interferograms (top: computed interferogram (Park90 model), bottom: experimental interferogram)

Figure 5.27: Comparison of interferograms (top: computed interferogram (Gupta model), bottom: experimental interferogram)
An important aspect associated with the process of molecular dissociation is the effect that dissociation has on the average vibrational energy of the molecules. Since the very energetic molecules are easily dissociated, it is clear that the dissociation process reduces the average vibrational energy remaining in the molecules. For the comparison of the preferential and nonpreferential model in Figs. 5.29 and 5.30, the effects of dissociation on vibration was modelled according to Treanor.
Computation of two dimensional flows

Figure 5.31: Interferogram: without and with effects of dissociations on vibrations (left and right figure respectively)

and Marrone as discussed in section 2.2.3.2. At higher shock strengths as in the present case, the process of dissociation has appreciable effect in lowering the vibrational temperature. The vibrational temperature increases slowly and the translational temperature does not fall rapidly. There is no cross over and overshoot of the vibrational temperature and the meeting of translation temperature and vibrational temperature is delayed until final equilibrium. When this effect of dissociation on vibration is neglected, an early approach of translational and vibrational temperature curves with a subsequent crossover point and overshoot in vibrational temperature over the local equilibrium value takes place. In Figs. 5.32 and 5.33, these aspects of vibration-dissociation coupling is clearly observed. The computed interferograms as shown in Fig. 5.31 indicates that, in conjunction with VT and VV model of Klomfaß and VD model of Treanor and Marrone, effect of dissociation on vibration should not be neglected.

In case of Treanor and Marrone’s model, the effect of vibrational relaxation on dissociation is included through a vibrational coupling factor $V$ which is described in detail in section 2.2.3.2. To take into account the same effect, Park proposed the evaluation of the dissociation rate coefficient at an average temperature using the translational and vibrational temperature. This model is also described in detail in section 2.2.3.1. At high temperature, Park’s model causes a high dissociation rate, which in turn results in smaller shock stand-off distances compared to Treanor and Marrone’s model, as is evident in Figs. 5.35 and 5.36. The corresponding interferograms are compared in Fig. 5.34. At low temperature range, both models show a reaction induction zone during which the dissociation is greatly inhibited by the lack of population of the higher vibration levels. The extent of the reaction induction zone is more pronounced with the Park model, thus, reducing the dissociation rate. Thus at a low temperature range, the shock stand-off distance can be larger in case of Park’s model than the
model of Treanor and Marrone.

The modelling of the vibrational relaxation time according to Klomfaß and Millikan and White was described in section 2.2.4.1. At high temperatures, the modelling of Millikan and White causes shorter relaxation times than Klomfaß. This in turn results in a sharp increase in the vibrational temperature due to a high rate of translational-vibrational energy exchange. A sharp increase in vibrational temperature leads to a high dissociation rate, which in turn results in a rapid fall of the translational temperature and sharp rise in density. Thus the shock stand-off distance is considerably smaller for the Millikan and White model as is evident in Figs. 5.38 and 5.39. The computed interferograms are compared in Fig. 5.37, which clearly shows the differences in the flow field using the two models. The shock stand-off distance varies by nearly 8%. In both cases, the preferential dissociation model of Treanor and Marrone is considered. The comparison between the preferential and nonpreferential dissociation model using the Millikan and White model is shown in Figs. 5.40 and 5.41. The influence of dissociation models on the shock stand-off distance is to be clearly observed. Similarly if the influence of dissociation on vibration is neglected, the difference in the shock stand-off distance, crossover and overshoot of vibrational temperature is observed, as is evident in Figs. 5.43. The computed interferograms as shown in Fig. 5.42 confirm these observations for the whole flow field. In all the computations for this test case, the model of Millikan and White was used with Park correction.

Comparing the computed interferograms with experimentally obtained interferogram, it is observed that the Park(90) reaction set in conjunction with the Treanor and Marrone VD coupling, and Klomfaß VT model (see Fig. 5.26), produces the flow field in quite good agreement. On the other hand, when the VT model of Millikan and White is used, the disagreement with the experiment is seen
Figure 5.34: Interferogram: Park model (left figure) and Treanor and Marrone model (right figure)

Figure 5.35: Temperatures along the stagnation line

Figure 5.36: Density and atomic nitrogen mass fraction along the stagnation line
5.3 Nitrogen flow over a circular cylinder

Figure 5.37: Interferogram: Klomfaß model (left figure) and Millikan and White model (right figure)

Figure 5.38: Temperatures along the stagnation line

Figure 5.39: Density and atomic nitrogen mass fraction along the stagnation line
Figure 5.40: Temperatures along the stagnation line

Figure 5.41: Density and atomic nitrogen mass fraction along the stagnation line

Figure 5.42: Interferogram: Millikan and White model without and with the influence of dissociation on vibration (left and right figure respectively)
5.3 Nitrogen flow over a circular cylinder

Figure 5.43: Temperatures along the stagnation line

Figure 5.44: Density and atomic nitrogen mass fraction along the stagnation line

(compare Fig. 5.37 (right figure) with Fig. 5.24). This may lead to giving preference to the VT model of Klomfaß over Millikan and White’s model. But as it will be seen in Figure 5.47, this conclusion is far from true. Figures 5.45-5.47 show the Navier stokes calculation of the same test case. The cylinder wall is assumed to be noncatalytic with a constant wall temperature of 300 K. The chemical reaction sets of Park(85) in conjunction with Park’s averaged temperature model to calculate the reaction rates and Millikan and White’s VT model, is used for this calculation. The effect of dissociation on vibration is neglected. Figures 5.45-5.46 show the variation of temperatures, and density and atomic nitrogen mass fraction, respectively, along the stagnation line. The relatively cold wall produces a temperature boundary layer with large temperature difference. The chemical composition of the gases at the wall is taken as same as just before the wall due to noncatalyticity of the wall boundary condition. This results in sharp concentration gradients near the wall. The comparison of computed interferogram with the experimental interferogram as shown in Fig. 5.47, show quite good agreement in the shock stand-off distance and the flow field. The bow shock is not resolved as fine as in the case of Euler calculation, since here only two adaptations were made with an initial grid of around 3500 cells. The final grid has about 13000 cells. There would be little variation in the shock stand-off distance with further adaptation. Since the purpose of the computation was to see the influence of a particular set of models on the shock stand-off distance and the overall flow field, further adaptation was not attempted.

In section 2.2.2, it was discussed that at high temperatures, there is a significant disagreement between reaction rates produced by different reaction sets. To minimize the uncertainty of the deviations in the reaction rates, a curve-fit was made using the existing chemical reaction models. An interferogram made out of this new rate sets is compared with experimental interferogram in Fig. 5.48. For this
computation, the Treanor and Marrone VD coupling was used together with the Klomfaß VT model. As observed with other reaction sets, the shock stand-off distance here also agrees reasonably well with the experiment but the differences in the flow field are clearly seen. The idea of minimizing the uncertainty by making a curve fit does not seem to be an elegant approach at least for the present test case, since the very purpose of minimizing the uncertainty in chemical reaction sets is far from any conclusion. This new reaction rate set may be suitable for a different test case. Thus with so many uncertainties in physiochemical modelling, it is not justified to make a judgment regarding the correctness of one model over another one which have been used in this work. By selecting a proper set of model sets, an experimentally obtained flow field can be reproduced by a suitable numerical simulation. At the same time, it is also inferred that the reliance on CFD calculation can not be made with confidence as far as thermochemical nonequilibrium is concerned.

5.4 Inviscid air flow over a sphere

The shock stand-off distance on spheres in hypersonic flow is one of the most appropriate parameter for validating the CFD results. Since for high Mach number flows on spheres, the shock stand-off distance is much smaller than the body radius, its experimental determination is difficult and large errors have to be accepted. Some significant theoretical studies have been made to predict the shock stand-off distance on spheres in hypersonic flow [68], [77], [103], [114].

For the non-reactive case, Lobb [68] performed extensive experiments on spheres in a ballistic range facility and measured the shock stand-off distance by schlieren photography. The comparison of his
results with Van Dyke's numerical solution, can be approximated quite well by [68]

\[
\frac{\Delta r}{D} = 0.44 \frac{\rho\infty}{\rho_0},
\]

(5.3)

where \( \Delta r \) is the shock stand-off distance, \( D \) is the sphere diameter and \( \rho_0, \rho\infty \) are the density immediately behind the shock and free-stream density, respectively.

Recently Olivier [77] developed a theoretical model to determine the shock stand-off distance on axisymmetric blunt bodies for frozen and equilibrium flows. This approach is based on the solution of the governing conservation equations and does not make use of previous results like Van Dyke's solution for blunt-body flows. This theory gives the following analytical solution for the shock stand-off distance:

\[
\Delta = \left\{ \frac{\partial r}{\partial \theta} \left[ \frac{1}{2} \left[ \frac{1 + \left( \frac{\rho\infty}{\rho_0} \right)^2}{\rho_0} \right] - \frac{1}{\gamma - 1} \frac{\partial \rho}{\partial \theta} \left[ \frac{1 + 2 \left( \frac{\rho\infty}{\rho_0} \right)^2}{\rho_0} \right] - \frac{1}{\gamma - 1} \left[ 1 + \frac{\rho\infty}{\rho_0} \right] \right] \frac{\rho_0 + \rho\infty}{\rho_0} \right\}
\]

(5.4)

The tangential velocity gradient, \( \frac{\partial \phi}{\partial \theta} \), is given as follows [2], [77]:

\[
\frac{\partial \phi}{\partial \theta} = \sqrt{2 \left( 1 - \frac{2}{\gamma + 1} \left( 1 - M_\infty^2 \right) \right)}, \text{ for frozen flow}
\]

(5.5)

\[
\frac{\partial \phi}{\partial \theta} = \frac{1}{2} \sqrt{\frac{\partial \phi}{\partial \theta}}, \text{ for equilibrium flow.}
\]

(5.6)
The solution for the frozen case agrees very well with the well-known solution of Van Dyke. For larger reaction rates and the limiting case of equilibrium flow, very good agreement is achieved with the approach of Wen and Hornung [77], [114].

In the present study, the computations of hypersonic inviscid air flow over a sphere were carried out for calorically perfect, chemical nonequilibrium and thermochemical equilibrium flow conditions. The free stream conditions are given in Table 5.3.

The sphere has a diameter of 0.0762 m. Figure 5.49 shows the computed iso-density plots. Figures 5.50 and 5.51 show the density and temperature distributions along stagnation line, respectively. The shock stand-off distance becomes larger as the flow condition is changed from equilibrium to calorically perfect gas case, as it was for the cylinder case. The temperature in the shock layer is significantly lowered by chemical reactions. The shock stand-off distance as given by the theoretical models for calorically perfect and equilibrium gas models are shown in Fig. 5.51. The agreement between the theoretical models and the present computation is quite good. The computed post normal shock temperature for the calorically perfect and equilibrium gas model are also presented in Table 5.4. The agreement between computed and analytical values is excellent.

<table>
<thead>
<tr>
<th>$\rho_0 [\text{kg/m}^3]$</th>
<th>$T_0 [\text{K}]$</th>
<th>$M_\infty [-]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0010269</td>
<td>270.65</td>
<td>10.07</td>
</tr>
</tbody>
</table>

Table 5.3: Free-stream conditions for air flow over a sphere

<table>
<thead>
<tr>
<th>Gas model</th>
<th>$T_{S\text{comp}}$</th>
<th>$T_{S\text{analytical}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calorically Perfect</td>
<td>5604 K</td>
<td>5595 K</td>
</tr>
<tr>
<td>Thermochemical Equilibrium</td>
<td>3221 K</td>
<td>3170 K</td>
</tr>
</tbody>
</table>

Table 5.4: Comparison of post shock temperature
5.4 Inviscid air flow over a sphere

Figure 5.49: Iso-Density plots (left: calorically perfect, center: chemical nonequilibrium, right: thermochemical equilibrium)

Figure 5.50: Density distribution along the stagnation line

Figure 5.51: Temperature distribution along the stagnation line
Chapter 6

Shock-on-shock interaction in hypersonic viscous flow

6.1 Introduction

The flow about a hypersonic vehicle is generally characterized by the occurrence of intense shock waves that form around its nose, ahead of the blunt leading edge of a wing, or around a deflected control surface. The existence of such shocks, which produce a very large increase in pressure and temperature levels, constitutes the most typical feature of hypersonic flow, and can be the source of mutual interaction or interference. Shock wave interference heating is a critical problem in the structural design of the thermal protection system and the load-carrying structure of high-speed vehicles. Extremely high-pressure and heat-transfer-rate gradients can occur in highly localized regions where interference pattern impinges on the surface. The extreme heat-transfer rate and gradients that occur over this narrow impingement region result in large temperature gradients and their attendant thermal stresses which limit the useful life of the structural component. In case of airbreathing propulsion, the phenomenon is typically located at the intake cowl lip, where the shocks produced by the compression ramps intersect the bow shock ahead of the cowl, but in general, it may affect in a similar manner the wing or the fin leading edge also. One of the first in-flight confirmations of the severity of shock-impingement heating occurred in October 1967, when the X-15A-2 suffered severe damage to its vertical fin (pylon) during a high altitude flight at Mach 6.7 (see Figs. 6.1-6.2) [111], [113]. Some of the practical examples are shown in Fig. 6.3. Figure 6.3(a) represents a ram-jet inlet with the shocks impinging on the cowl lip, Figure 6.3(b), the bow shock produced by an aircraft fuselage impinging on a wing or fin leading edge and Figure 6.3(c), the bow shock from the main body of a missile impinging on a side-strapped booster or fuel tank. Vehicles such as these operate in regimes that produce significant departures from thermochemical equilibrium in the flow about vehicle surfaces. Improved understanding of the influence of real gas effects on the shock interaction phenomenon reduces a significant element of risk in the design of hypersonic vehicles.
6.1 Introduction

Figure 6.1: Ram jet model mounted on vertical fin of X-15A-2 aircraft prior to test flight [25]

Figure 6.2: Side and front view of vertical fin showing damage due to shock impingement [25]

Figure 6.3: Practical examples of shock impingement heating
6.2 Shock-wave interference patterns

A detailed flow field structure is required to predict the magnitude of the aerodynamic heating rate in such a flow field. The first step in determining the effects of shock impingement on the pressure and heat-transfer rate is to determine the interference pattern that will exist when two oblique shocks of different strength intersect. The type of interference pattern obtained is dependent on the relative strength of the intersecting shocks and the geometry of the body on which the extraneous shock will impinge. Many researchers have investigated the shock-on-shock interference heating during the past decades, both experimentally and numerically. The most complete description of the shock impingement phenomenon is due to Edney [25], who observed and categorized six distinct shock-wave interference patterns known as types I-VI, all of which can occur when an oblique shock intersects the bow shock of a leading edge (Fig. 6.4). Three of the interference patterns (I, II, and V) result in shock-wave/boundary-layer interactions. Type III results in an attaching shear layer, and type VI results in an expansion-fan/boundary-layer interaction. Type IV is characterized by an impinging or grazing supersonic jet. Each interference pattern is discussed in detail by Edney [25]. The present study mainly concentrates on type IV interference pattern, since the heating rates for remaining regimes are less intense and therefore not design limiting. Some of the investigations in the present work exhibit the type III interference patterns. Therefore, a brief description of the features of the type III and type IV interference patterns is given subsequently in this section.

6.2.1 Type III interference pattern

A type III interference pattern occurs when a weak incident shock intersects a bow shock inside the subsonic region near the sonic point as shown in Fig. 6.5. The flow in the region above the shear layer (region 2) is subsonic, and the flow between the shear layer and the transmitted shock (region 4) is supersonic. The flow in regions 2 and 4 are at the same pressure and are turned at the same flow angle. Depending on the angle, the shear layer makes with the tangent to the body surface, the shear layer
will be undeflected and attached to the surface. The supersonic flow is deflected downward through an oblique shock, the strength of which depends on the Mach number and the flow turning angle. Pressure and heat-transfer-rate amplification caused by the attaching shear layer is analogous to a reattaching separated boundary layer. The state of the shear layer (laminar or turbulent) is a critical parameter in determining the pressure and heat-transfer rates.

### 6.2.2 Type IV interference pattern

The type IV interference pattern occurs when an oblique shock wave intersects the nearly normal portion of the bow shock from a blunt leading edge as shown in Fig. 6.6. The non-linear interaction of the shock waves results in the further displacement of the bow shock and the formation of a supersonic jet contained between two shear layers and submerged within the subsonic shock layer between the body and the bow shock wave. This inviscid jet formation process is local in nature and is independent of the interaction of the jet with the body. Referring to Fig. 6.5, when the wall turning angle is greater than the maximum turning angle for region 4 to produce the supersonic flow in region 5, the type III interference transitions to type IV. The flow process upto region 4 is identical to the type III interference. However, for the type IV interference, supersonic flow in region 4 is turned through a weak left-running wave to region 6. The flow in region 6 matches the flow direction and pressure with the subsonic flow in region 5. Supersonic flow in region 6 is brought to region 7 through a series of expansion and compression processes. A jet bow shock is produced when the jet impinges on the surface, creating a small region of high stagnation heating. A portion of the jet passes both above and below the cylinder and so the stagnation streamline must pass through the supersonic jet. The maximum pressure and heat-transfer rate occur when the jet impinges perpendicular to the surface. Whilst the stagnation enthalpy is conserved along all the streamlines in steady flow, the entropy is lower for streamlines that pass through the relatively weak jet shock system than for the streamlines that pass through the adjacent strong bow shock waves. Elevated surface pressures are produced at the base of the jet since both pressure and density increase as entropy decreases at constant enthalpy. The elevated density and the strong velocity gradients produced by the impingement of the supersonic jet provide the mechanism for locally increased heat transfer.

### 6.3 Real gas effects

In various spaceflight applications, be it winged or ballistic entry into planetary atmospheres, be it powered ascent to orbital flight or exploratory missions that traverse planetary atmospheres, the aerodynamic design of a vehicle’s performance has to consider real gas effects. In particular, the desire to build vehicles capable of flying to low earth orbit in single stage using air breathing engines and utilizing aerodynamic lift, challenges our understanding of real gas effects occurring both in aerodynamics and combustion [27]. For the case of a vehicle travelling at near orbital speeds, the Mach number is large and strong shock waves will be dominant features of the flow. The specific kinetic
Shock-on-shock interaction in hypersonic viscous flow

Figure 6.5: Type III interference pattern

Figure 6.6: Type IV interference pattern
energy for a vehicle in low earth orbit at a velocity of 8 km/s is 32 MJ/kg. Oxygen and nitrogen dissociates completely at specific energies of approximately 17 MJ/kg and 34 MJ/kg respectively [88] and so strong dissociation will occur in the flow about the vehicle. The phenomena of dissociation and vibrational excitation occur as a result of two-body collisions. The production of vibrationally excited molecules and the production of atoms from diatomic molecules are proportional to the number density of the original species. The recombination reaction, however, requires the presence of a third collision partner, and, is proportional to the square of the density of the original species. The primary effect of dissociation reactions on high enthalpy blunt body flows is to increase the density of the gas in the shock layer, which in turn, results in reduced shock stand-off distance. This effect influences the length scales of the flow field around the vehicle. In the nonequilibrium flow regime, a thermochemical length scale is introduced into the problem. Variations in the relative magnitudes of the thermochemical and fluid mechanical length scales introduce effects that are not encompassed by perfect gas models [50], [51].

As discussed in section 6.2, the large heating and pressure loads developed in the regions of shock-shock interaction results principally from an efficient recompression process, where the gas in the stagnation region is processed through a series of shock patterns. This is particularly true for the type IV shock-shock interaction where the flow is processed through a series of shocks terminating in a stagnation region preceded by a strong normal shock. It is the sensitivity of the shock patterns to the local which led Edney [25] to speculate that the heating rates developed in these flows would be more severe as a result of real gas effects. By mapping the type IV flow field into the pressure-deflection plane, Edney [25] was able to compute the variation of the pressure at the jet-impingement point for various free-stream conditions. Significant real gas effects were suggested by the increase in the peak pressure with decreasing ratio of specific heats.

In type IV flow, the three shock waves at the two triple points, produce widely differing dissociation levels and reaction lengths due to their disparate shock strengths and are therefore expected to produce strong nonequilibrium effects. Shear layers that are generated at the triple points cause energy release by mixing the dissociated low-speed fluid with the lower temperature supersonic fluid and this probably influences the shear layer density and spreading rates. Thus influence of turbulence-chemistry interaction will become important when the type IV jet width is small relative to the shock standoff distance so that turbulent diffusion processes consume the inviscid type IV jet core [88]. Similar but lesser effects might be expected for the type III interaction region, where the real gas effects might be expected to influence the aerothermal loads in the reattachment region of the free shear layer [49].

Sanderson [88] describes the real gas effects on the viscous flow in the boundary layer that forms at the jet impingement point. Jet impingement greatly increases the recombination rates in the boundary layer since these scale with the square of the density intensification at the jet impingement point. In the immediate vicinity of the jet impingement point, the behaviour parallels that of the classical blunt body problem.
Fay & Riddell [28] showed that when the recombination rate in the boundary layer is large,

\[ \dot{q} \sim \sqrt{\frac{1}{\rho_e \mu_e} \frac{d \mu_e}{d \rho}} \]  

(6.1)

Here \( \dot{q} \) is the heat transfer rate per unit area and time, \( \rho_e, \mu_e \) and \( \frac{d \mu_e}{d \rho} \) are the density, viscosity, and transverse velocity gradient respectively at the outer edge of the boundary layer. The most important real gas influences on the stagnation point flow are the increased density of the outer flow and the coupled effect on the velocity gradient at the edge of the boundary layer. A broad range of possible influences arise as a consequence of the strong interdependence of real gas effects and density.

6.4 Review of previous work

Following the work of Edney [25], the problem of shock-shock interactions has been addressed with experimental, theoretical and computational efforts.

Several investigators have attempted analytical solutions of the flow field. Edney [25] and Morres and Keyes [72] used oblique shock and Prandtl-Meyer expansion relationships to predict the interference pattern and peak pressure and peak heat transfer rate, with good success. However their methods rely on experimental measurements of the shock stand-off distance and transmitted shock length [116]. Tannehill et al. [98] produced one of the earliest attempts to understand such a flow field. Recent numerical studies include Klopfer and Yee [57], Lind and Lewis [63], Zhong [119], Thareja et al. [100], Vegamanti [107], Gaitonde and Shang [31], Glass [32], Ambrosio [1], etc. These studies employ a range of numerical algorithms including finite-difference, finite volume implementations, unstructured adaptive meshing techniques using triangular cells, etc. Tannehill et al. [98] first computed time-accurate shock-shock interference heating problems using a time accurate second-order MacCormack scheme. Because the shear layer and the embedded shock are captured with a relatively coarse set of grids, some of the detailed structure of the interference flow field is lost. Klopfer and Yee [57] used the second order implicit TVD schemes to obtain steady-state solutions. In their computations of a type IV interference flow field, convergence rates were slow due to the unsteadiness of the flow and the impinging shock did not converge to a fixed location. Thareja et al. [100] used an upwind finite element technique with adaptive triangular grids to compute the interference heating flow. Their computations also experienced unsteadiness in computing steady-state type IV interference heating flow. Glass [32] made a time accurate computation of low-density, Mach 10 shock-wave interaction tests, performed at ONERA R5Ch hypersonic tunnel and observed that the flow is steady after an initial transient to establish the shock interaction, which occurred within 10 \( \mu s \). Jet oscillations appeared in the computations of Gaitonde [31], where limit-cycle oscillations were observed in the computational residual as the mesh resolution was increased. Gaitonde [31] addressed the issue of time-accuracy of the algorithms that were used and concluded that the oscillations were attributable to the physics of the problem. Zhong [119] used high order, finite volume, essential non oscillatory scheme (ENO) to study the type IV shock interaction and concluded that the inherent unsteadiness...
is the result of the interaction among the unsteady shear layers and the bow shocks. Lind and Lewis [63], [64] demonstrated via time-accurate simulations, that the apparent unsteadiness of the type IV interaction is related to the formation and shedding of shear layers within the shock layer and acoustical feedback between the distorted bow shock and the body. Ambrosio [1] discussed the issues related to the use of correct boundary conditions behind the impinging shock, grid convergence, and time unsteadiness of CFD simulations. He concluded that the strong tangential grid refinement is necessary to capture accurately the very narrow pressure and heat flux peaks. Regarding the boundary condition, his observation was that sometimes imposing Rankine-Hugoniot relations for evaluating the impinging shock strength is an inadequate procedure considering the influence of hypersonic viscous interaction on the impinging shock characteristics. He observed that the time unsteadiness could be due to an inherent time dependent character of the supersonic jet and to the presence of disturbances in the wind-tunnel flow. Most of these numerical studies, however, assumed a perfect gas model in high Mach number free-streams. Following the empirical predictions of Edney [25], for real gas effects in regions of shock-shock interaction, a number of studies have been attempted to quantify these effects. The effect of finite-rate chemistry was considered by Hannemann et al. [40] and Brück [15] who simulated the experimental results of Kortz [58] and Kortz et al. [59]. These computations indicated the persistence of the type IV behaviour for shock-impingement locations intermediate to those discussed by Kortz, and indicated a suppressed reaction rate in the impinging jet fluid. Carlson and Wilmoth [17] used a direct simulation Monte Carlo (DSMC) technique in conjunction with nonequilibrium air chemistry to compute the type IV interference heating flow in a continuum flow regime. They found that the grid size and selection had a significant effect on the solution and that careful gridding in the base of the interaction region was of critical importance to the accurate prediction of the heating levels. Their results indicated that the real gas effects can result in almost doubling the peak pressure levels in the interaction, and the peak heating levels are increased by approximately 150 percent when real gas effects are present. A similar set of predictions were made by Furumoto and Zhong [29] for continuum real gas flows. In another numerical study of type IV shock-shock interactions of pure $N_2$ flow over a cylinder, Furumoto et al. [30] found that real gas effects reduce the level of peak surface heating and peak surface pressure due to endothermic real gas effects. Lee [62] investigated the effects of thermochemical nonequilibrium phenomenon on type IV shock-shock interaction flow fields and found that the local maximum pressure and heat flux are about 10 times larger than those without shock-shock interactions. Hannemann [42] made a detailed study of shock-shock interactions with a time accurate code, with varying position of the impinging shock on the bow shock. He found that the maximum heating level could go up to 30 times than those without shock-shock interactions and this maximum heating occurs for a case which lies between type III and IV interference flow patterns. Keuk et al. [105] made steady state computations of Sanderson’s experiments [88] of type IV shock interference flow fields and found that the computed peak heat transfer lies below the experimental values. The possible cause of this disagreement may be an insufficient grid resolution as strong grid refinement is required to resolve the flow features in case of a shock-shock interaction.
Craig and Ortwerth [21] experimentally measured pressures and heat transfer rates on a cylindrical leading edge typical of a hypersonic inlet cowl. However, large instrumentation resulted in poor resolution of the peak pressure and heat transfer. The experiment performed at ONERA R5Ch hypersonic wind tunnel [83] produced various shock-wave interference patterns, depending on the relative position of the incident and bow shock wave. Wieting and Holden [116] conducted an experimental study and obtained data detailing the influences of the Reynolds number, Mach number and incident shock strength at modest enthalpies. Recently, few experimental studies have been conducted to investigate the influence of real gas effects on the structure and aerothermal load generated in regions of shock-shock interaction. Kortz [58] and Kortz, MacIntyre and Eitelberg [59] report experimental investigations conducted at enthalpies sufficient to cause significant nitrogen dissociation in the DLR HEG free-piston shock-tunnel. This work included the first quantitative interferometric visualization of shock impingement flows. Elevated heat transfer rates were not observed for the range of parameters that were investigated and this appears to have resulted from a relatively coarse variation of the shock impingement location. Sanderson [88] concluded as a result of experimental studies conducted in the T5 piston-driven shock tunnel that the real gas effects cause an increase in the scale of the interaction region which results in a reduction in the peak heating enhancement. Sanderson discusses about the development of an improved model to elucidate the finite-rate thermochemical processes occurring in the interaction region and concludes that the model accurately predicts the measured heat transfer rate. In the studies conducted by Holden [48], measurements were made in regions of shock-shock interaction at enthalpy levels of 5 and 10 MJ/kg for both air and nitrogen flows. The measurements indicate that while real gas have a minor influence on pressure, the heat transfer rates are larger in the air flow.

6.5 Results and Discussions

In this section, results are presented for a series of numerical simulations of experiments conducted in the GALCIT T5 free piston driver shock tunnel [88] to determine the quantitative effects of high enthalpy thermochemistry on the shock impingement heating problem. In the experiment, the flow topology was simplified by studying the nominally two-dimensional flow about a cylinder of diameter 40.6 mm with a coplanar impinging shock wave. A large shovel-shaped shock generator was used to produce a planar oblique shock wave with uniform downstream flow. Variations in the shock impingement flow field were produced by vertically translating the cylinder model with respect to the exit of the shock generator. The shock generator was inclined at an angle of 6 degrees for all the experiments, which were numerically simulated in the present work. Holographic interferometry was used to visualize the flow field and to quantify the increases in the stagnation density caused by shock interactions. Time-resolved heat transfer measurements were obtained from surface junction thermocouples about the model forebody.

Three different test conditions were used which are summarized in the Table 6.1. The first test condition, case A, represents a low enthalpy control condition where the only real gas effects are a partial
excitation of the vibrational modes in the stagnation regions of the flow. Case C represents a high enthalpy condition that was chosen to highlight the influence of nonequilibrium thermochemistry on the problem. Case B is an intermediate enthalpy condition that was designed to aid interpretation of the differences in the flow mechanisms for cases A and C. Nitrogen test gas was used for all the experiments.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\rho_\infty$ [kg/m$^3$]</th>
<th>$V_\infty$ [m/s]</th>
<th>$T_\infty$ [K]</th>
<th>$X_{\text{N}_2}$</th>
<th>Stanton Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A</td>
<td>0.0218</td>
<td>2540</td>
<td>162</td>
<td>1.0</td>
<td>0.0123</td>
</tr>
<tr>
<td>Case B</td>
<td>0.0155</td>
<td>4450</td>
<td>1190</td>
<td>0.99</td>
<td>0.0172</td>
</tr>
<tr>
<td>Case C</td>
<td>0.0157</td>
<td>5350</td>
<td>2326</td>
<td>0.95</td>
<td>0.0167</td>
</tr>
</tbody>
</table>

Table 6.1: Free-stream conditions and theoretical stagnation point Stanton number for the test cases

6.5.1 Flows without shock-shock interaction

The flow about the cylinder without shock wave impingement was numerically simulated for the test cases A, B and C. It was found that the grid adaptation causes some problems due to the occurrence of hanging nodes in the boundary layer. Therefore for these simulations, grid adaptation is not used. The adverse effect of grid adaptation is presented with one simulation for case C. The numerical accuracy of the results are estimated by a grid refinement study for test case B. In the presented results, the heat transfer data have been reduced to Stanton number form and normalized with respect to the predicted stagnation-point value according to Fay \& Riddell [28]. The values for the predicted stagnation-point Stanton number without shock impingement at each test condition are given in Table 6.1. Unless otherwise mentioned, the computations were made with the reaction rates model of Park 85 [79] and the Riemann solver of Roe [87] extended for chemically reacting gases [67].

Figure 6.7 presents surface Stanton number distributions for three different meshes for case B. The computation using two meshes with number of cells 14400 and 19600, respectively converge to nearly the same Stanton number distribution. The computed surface Stanton number distribution is compared with the experimental result of Sanderson [88] in Fig. 6.8. The agreement between experiment and computation is excellent. A comparison of the computed interferogram with the experimental interferogram is presented in Fig. 6.9. The interference fringes behind the shock agree with experiment. The present code computed a fringe shift at the boundary layer edge near the stagnation point of 10.7 while the experimental fringe shift reported by Sanderson is 10.5. However the disagreement between the present computation and the experiment with regard to the shock stand-off distance is clearly to be seen. The difference in shock stand-off distance between computation and experiment was also observed by Furumoto et al. [29]. They pointed out referring the work of Olejnizczak et al. [76] regarding the comparison of the computational results of double wedge experiments in T5, that the free stream of the test section is not in thermal equilibrium. Figures 6.10 and 6.11 present the comparison of the computed density and molecular nitrogen distributions with the computation performed by van Keuk et al. using the FLOWer-CNE code [105]. The agreement regarding the shock stand-off distance and the length and shape of the relaxation zone is quite good.
Additionally Fig. 6.12 shows the comparison of density distributions computed by van Keuk et al. using the FLOWer-CNE [105] and Candler’s code [16]. This comparison also shows quite satisfying agreement regarding the shock stand-off distance. It is observed that the different CFD codes agree on the shock stand-off distance for this test case. Thus it can be concluded that the disagreement regarding the shock stand-off distance between the present computation and the experiment may be due to an uncertainty in the free stream conditions. Sanderson [89] also mentions that the flow in the nozzle is predicted to exhibit some angularity and Mach number non-uniformity at the low enthalpy off-design conditions A and B. A proper estimation of free stream condition is necessary for a better agreement between computational and experimental results. Figure 6.13 presents a comparison of the computed surface Stanton number distribution with the experiment of Sanderson [88] for case C. Again excellent agreement between computation and experiment is obtained. The amount of artificial viscosity introduced by different upwind methods has significant influence on a sensitive quantity like heat flux, as shown in Fig. 6.14. The interference fringes behind the shock agree well with the experiment (see Fig. 6.15). The present code computed a fringe shift at the boundary layer edge near the stagnation point of 10.2, while the experimental fringe shift reported by Sanderson is 9±1. Figures 6.16 and 6.17 present the comparison of the computed density and molecular nitrogen distributions with the computation performed by van Keuk et al. using the FLOWer-CNE code [105]. Additionally, Fig. 6.18 shows the comparison of density distributions using the Flower and Candler’s code. The agreement among different CFD codes, regarding the shock stand-off distance is quite good. Unlike case B, the present computation differs with the FLOWer-CNE code in the prediction of the relaxation length. This could be due to the different thermochemical modellings used in the two codes, which significantly influences the relaxation processes at high enthalpy condition. The disagreement with the experiment regarding the shock stand-off distance may be again related to an incorrect determination of the free stream conditions. For this test case, computations were also performed with grid adaptation. Figure 6.19 shows the Stanton number distribution on adapted grids.
6.5 Results and Discussions

Figure 6.9: Comparison of interferograms for case B (upper half: computational, lower half: experimental)

Figure 6.10: Comparison of density distribution for case B (upper half: QUADFLOW, lower half: FLOWer-CNE [105])

Figure 6.11: Comparison of molecular nitrogen distribution for case B (upper half: QUADFLOW, lower half: FLOWer-CNE [105])

Figure 6.12: Comparison of density distribution for case B (upper half: Candler code, lower half: FLOWer-CNE [105])
The influence of occurrence of hanging nodes in the boundary layer is clearly seen in the form of a non smooth variation of the Stanton number profile. It was for this reason that the test cases without impingement shock were computed without adaptation for a better comparison with the experiment. The grid adaptation has no effect on the $C_p$ distribution as shown in Fig. 6.20. Thus surface pressure is not a sensitive quantity to be used for code validation purpose.

Finally for case A, the comparison between computational and experimental interferogram is shown in Fig. 6.21. The computation was made with frozen flow assumption. The shape of the fringes behind the bow shock confirms the frozen flow behaviour of the flow. Though the interferogram fringes do not agree just behind the bow shock, the agreement regarding fringe shift at the boundary layer edge near the stagnation point is quite satisfying. The present code computed a fringe shift at the boundary layer edge near the stagnation point of 11.4, while the experimental fringe shift reported by Sanderson is 13±1. The disagreement between the present computation and the experiment with regard to the shock stand-off distance is clearly to be seen. The disagreement regarding fringe shapes behind the bow shock could be due to the factors as mentioned earlier. The agreement between computation and experiment regarding the surface Stanton number distribution is again quite good (see Fig. 6.22).

The disagreement between computation and experimental results regarding the shock stand-off distance and the density distributions in the shock layer were also reported by Kastell et al. in the context of some other test cases [53]. For CFD validation purposes, the free stream conditions (including flow gradients and quality) must be known accurately [7], [18], [41], [53]. The free-stream conditions in high-enthalpy facilities are very difficult to determine to very high accuracy. Non-equilibrium nozzle calculations are still difficult; the same holds for experiments [53]. The shock stand-off distance is quite sensitive to variations in the free-stream conditions, in particular to the degree of dissociation. A higher degree of dissociation in the free-stream leads to a lower density jump $\rho_f/\rho_{in}$ at the frozen shock wave front and thus to a larger shock stand-off distance. Hannemann et al. [41] made computations of the flow over the cylinder in two and three dimensions, respectively and compared the results with the experiments conducted in HEG. One aspect of their investigations was to study the influence of the flow past the edges of the cylinder on the flow in the central part of the model. They applied averaged parallel as well as conical flow conditions, which corresponded to the flow in the test section of the nozzle. They found that for the comparison of flow quantities measured in the central part of the cylinder (e.g. surface pressure or heat flux), two dimensional flow computations are sufficient. However, when comparing measured and computed interferograms, three dimensional flow computations are necessary. The use of the conical flow in the test section as an inflow condition for the three dimensional case affects the numerical phase shift distribution in the flow field, while having little impact on the surface pressure and heat flux in the center plane of the cylinder. The 3d effects of holographic interferometry in the experiment is also pointed out by Kastell et al. [53]. Considering the observations made by several authors, similar conclusions can be made regrading the disagreement between the present computational and experimental interferograms. In particular the disagreement between computational and experimental interferograms (Fig. 6.21) for case A is quite interesting to observe. The computational interferogram shows a completely frozen
6.6 Flows with shock impingement

The main aim of the present study is to investigate the effects of nonequilibrium thermochemistry on the Edney type IV interaction, since it causes locally intense enhancement of the heat transfer.
Figure 6.17: Comparison of molecular nitrogen distribution for case C (upper half: QUADFLOW, lower half: FLOWer-CNE [105])

Figure 6.18: Comparison of density distribution for case C (upper half: Candler code, lower half: FLOWer-CNE [105])

Figure 6.19: Stanton number distribution on adapted grids for case C

Figure 6.20: $C_p$ distribution on adapted grids for case C
6.6 Flows with shock impingement

Figure 6.21: Comparison of interferograms for case A (upper half: computational, lower half: experimental)

Figure 6.22: Comparison of computed Stanton number distribution at the wall with the experimental data of Sanderson for case A

rate. Edney type IV configuration occurs when the shock impinges in the vicinity of the geometrical stagnation point. The peak heating and jet impingement location is sensitive to the shock impingement angle and shock strength. In the type IV interaction, a portion of the jet passes both above and below the cylinder and so the stagnation streamline must pass through the supersonic jet. In computational simulations, the location of the impinging shock wave should be adjusted to achieve a flow topology for which the stagnation streamline coincides with the mid point of the jet [88]. Therefore computationally, in order to simulate the shock-shock interaction flows, a spectrum of cases with different impinging shock locations was computed. Figure 6.23 shows schematically the variation of the shock impingement location on the vertical axis of the cylinder. Here h represents the vertical distance from the cylinder center point, non-dimensionalised by the radius of the cylinder. The post-impinging shock conditions are obtained using the Rankine-Hugoniot relations. In the experiment, the free stream conditions may exhibit non-uniformity and angularity which may result in shock angles which are slightly larger than those indicated by simple oblique shock relations [88], [89]. The shock angles and therefore the post-impingement shock conditions may also be influenced by the hypersonic viscous interaction on the shock generator. Sanderson [88], [89] provides the shock angles that form the best basis for data analysis. In the present work, computations were made for shock angles corresponding to a shock generator angle of $\alpha = 6^\circ$ as well as for corrected shock angles as suggested by Sanderson. The impinging shock angles corresponding to the shock generator angle ($\alpha = 6^\circ$) are 10.55°, 13.2° and 14.7° respectively. The corrected shock angles suggested by Sanderson are $14.25^\circ \pm 1^\circ$, $15^\circ \pm 1^\circ$ and $16^\circ \pm 1^\circ$ respectively. The assumption of laminar flow in chemical nonequilibrium but in thermal equilibrium were made in the computations. The reaction rates model...
of Park 85 [79] and the Riemann solver of Roe [87] extended for chemically reacting gases [67] were used. The assumption of a noncatalytic wall with a constant temperature of 300 K has been made at the body surface. The computations were performed with the grid adaptations. The problem of occurrence of hanging nodes near the boundary layer appear to be still there but due to a large refinement of the grid near the interaction region, this problem disappears, as will be shown in the surface Stanton number distributions.

### 6.6.1 Case A, shock angle $\beta = 10.55^\circ$

The computation started on an initial mesh of 5184 number of cells. Two adaptations were performed which looked quite sufficient to capture all the flow phenomena. However the solution is expected to change quantitatively with more adaptations (see Fig. 6.32). The number of cells for the second and third mesh varied for different $h$, which is 18777 and 22449 for $h = 0$ and $h = 0.19$ respectively. The computation is performed with explicit time integration employing local time stepping till the bow shock is properly resolved. Then the computation is restarted with global time stepping.

Figure 6.24 presents the Stanton number distributions for different values of $h$. The comparison of the computed surface Stanton number distribution with the experiment is shown in Fig. 6.25. Though the computed Stanton number distribution corresponding to $h = 0.1$ is in relatively better agreement with the experiment, it does not correspond to a type IV interaction. The comparison of the detailed flow field (see Fig. 6.26) in conjunction with the pressure contours (see Fig. 6.27), with the flow field pattern of type III and type IV as shown in Figs. 6.5 and 6.6, confirms that the interference pattern is like a transition pattern between type III and IV. The flow topology corresponding to $h = 0.14$ and $h = 0.19$ represents the typical type IV interference pattern. In both cases, the stagnation streamline passes through the center of the well developed supersonic jet, which is nearly normal to the surface, as shown in Figs. 6.28 and 6.29. The peak heating in the case of $h = 0.19$ is little higher than that for
6.6 Flows with shock impingement

Figure 6.24: Stanton number distribution for different values of $h$ for case A

Figure 6.25: Comparison of computed Stanton number distributions at the wall with the experimental data of Sanderson for case A

$h = 0.14$, which is also confirmed by the little closeness of the jet towards the body (see Fig. 6.40). The flow pattern is studied in detail for $h = 0.19$. Figure 6.30 shows the grids used for the computation for $h = 0.19$. The grid adaptation plays an important role in resolving the complex flow features associated with shock-shock interaction, as is evident from Fig. 6.31. The supersonic jet which is virtually non-existent on the initial mesh, develops significantly on the final mesh. The peak heating and the angular location of the jet impingement changes significantly with grid adaptation as shown in Fig. 6.32. The wave patterns inside the jet are completely described with the aid of Figs. 6.33-6.35. The supersonic stream passes through the embedded shock and expansion fan, which is evident from the pressure variations along the upper and lower stream lines. As the jet finally approaches the body, the supersonic stream that flows inside the jet is suddenly decelerated through a detached shock. The jet is finally divided into two streams, which flow upward and downward from the stagnation point. At this point, particles flow along both stream lines at subsonic speed. Another subsonic compression of the flow occurs between the detached jet shock and the stagnation point. From this analysis, the flow field inside the jet can be interpreted as shown in Fig. 6.6. Figures 6.36 and 6.37 present the variation of the peak Stanton number and the angular location of the jet impingement with the timesteps. The jet impingement location has come to a fixed angular point whereas the Stanton number has a cyclic variation. This shows that the jet is unsteady but of small amplitude. One possible reason of the jet unsteadiness could be the propagation of a pressure wave, generated by the interaction between the shock waves in the supersonic jet structure and the shear layer outside the jet, to the upstream direction through the subsonic shock layer. This results in the oscillation of the bow shock i.e., the stand-off distance keeps changing continuously. The cause of unsteadiness in this case is not the formation and shedding of vortices as found by some of the researchers like Lind [63] and Furumoto et al. [29]. The velocity gradients across the shear layer may not be sufficient enough for the vortices to be formed. The flow field corresponding to $h = 0$ and $h = 0.3$ is shown in Figs. 6.38 and 6.39, respectively. There is no formation of supersonic jet and the flow just sweeps along the lower and upper part of the cy-
linder surface respectively, for h = 0 and h = 0.3. Figure 6.41 shows the experimental interferogram and Figs. 6.42-6.44 present computational interferograms for h = 0.1, 0.14 and h = 0.19 respectively. None of the computational interferograms agree with the experimental interferogram. The possible causes for the disagreement could be the same as mentioned in section 6.6. The disagreement was also found for a computation performed with the FLOWer-CNE code [105]. Additionally the computational Schlieren pictures for the flow field corresponding to h = 0.1 and h = 0.19 are shown in Figs. 6.45 and 6.46 respectively. The Schlieren pictures provide the density gradient in the flow field which is suitable for identifying some vital informations like the location of shocks, shear layers, etc. The disadvantage associated with the Schlieren picture is that the information regarding shock layer compression of the flow field is difficult to identify, which is easily obtained in interferograms. The Schlieren pictures clearly show the presence of the shear layers and the jet shock and the transitional nature of the flow between type III and type IV interaction pattern for h = 0.1.

6.6.2 Case A, shock angle $\beta = 14.25^\circ$

The shock angle is increased to $14.25^\circ$ as proposed by Sanderson and correspondingly the post-impinging shock conditions are changed. The computational results, which correspond to h = 0.14, are shown in Figs. 6.47-6.52. The reason for the disagreement regarding interferograms is the same as mentioned earlier. The variation of the jet impingement angle and the peak Stanton number with time is more stronger than corresponding to a shock angle of $10.55^\circ$ and results in the formation of vortices as is evident in Fig. 6.51. The vortices do not follow a pattern of formation and shedding as some authors have found out [63], [119]. This is evident with not so significant variation in the
6.6 Flows with shock impingement

Figure 6.28: Details of the flow field for case A at \( h = 0.14 \), sonic line (dots), stream lines (solid)

Figure 6.29: Details of the flow field for case A at \( h = 0.19 \), sonic line (dots), stream lines (solid)

Figure 6.30: Sequence of grids used for case A at \( h = 0.19 \)
Figure 6.31: Comparison of the jet shape for all grids for case A at h = 0.19, geometry of sonic lines

Figure 6.32: Stanton number distribution for all grids for case A at h = 0.19

Figure 6.33: Pressure contours for case A at h = 0.19

Figure 6.34: Pressure variation along upper streamline for case A at h = 0.19
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Figure 6.35: Pressure variation along lower streamline for case A at \( h = 0.19 \)

Figure 6.36: Variation of peak Stanton number for case A at \( h = 0.19 \)

Figure 6.37: Variation of jet impingement angle for case A at \( h = 0.19 \)

Figure 6.38: Details of the flow field for case A at \( h = 0 \), sonic line (dots), stream lines (solid)
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Figure 6.39: Details of the flow field for case A at \( h = 0.3 \), sonic line (dots), stream lines (solid)

Figure 6.40: Comparison of jet shape for different values of \( h \) for case A, geometry of sonic lines

Figure 6.41: Experimental interferogram for case A

Figure 6.42: Computational interferogram for case A at \( h = 0.1 \)
6.6 Flows with shock impingement

6.6.3 Case B, shock angle $\beta = 13.2^\circ$

This test case represents a medium enthalpy condition where moderate chemical reactions will take place. Across the weak impinging shock, the composition of the gas will not change and therefore the post-impinging shock conditions were determined using the frozen flow assumption. As it was for case A, to accelerate the convergence, local time stepping was used on the initial mesh till the essential flow features were properly resolved and then the computation was restarted with global time stepping. The computation on the final mesh was continued till the peak Stanton number and its angular location approaches a nearly steady state. The computations were made with different values of $h$ to get a value which corresponds to type IV interaction. Like in test case A, the initial mesh consists of 5184 number of cells and the number of cells on the final mesh differs depending on $h$. The final mesh has 18798 and 21690 number of cells for $h = 0.1$ and $h = 0.234$ respectively. The surface Stanton number distribution corresponding to different $h$ is shown in Fig. 6.53. Figure 6.54
Figure 6.45: Computational schlieren picture for case A at $h = 0.1$

Figure 6.46: Computational schlieren picture for case A at $h = 0.19$

Figure 6.47: Computational interferogram for case A at $h = 0.14$ ($\beta = 14.25^\circ$)

Figure 6.48: Computational schlieren picture for case A at $h = 0.14$ ($\beta = 14.25^\circ$)
6.6 Flows with shock impingement

Figure 6.49: Variation of peak Stanton number for the final mesh for case A at $h = 0.14$ ($\beta = 14.25^\circ$)

Figure 6.50: Variation of jet impingement angle for the final mesh for case A at $h = 0.14$ ($\beta = 14.25^\circ$)

Figure 6.51: Details of the flow field at time $t_3$ (see Fig. 6.49) for case A at $h = 0.14$, sonic line (dots), stream lines (solid) ($\beta = 14.25^\circ$)

Figure 6.52: Comparison of computed Stanton number distribution for case A for the two shock angles
Figure 6.53: Stanton number distribution for different values of h for case B

Figure 6.54: Comparison of computed Stanton number distribution at the wall with the experimental data of Sanderson for case B

Figure 6.55: Details of the flow field for case B at h = 0.1, sonic line (dots), stream lines (solid)

Figure 6.56: Details of the flow field for case B at h = 0.15, sonic line (dots), stream lines (solid)
6.6 Flows with shock impingement

Figure 6.57: Details of the flow field for case B at $h = 0.234$, sonic line (dots), stream lines (solid)

Figure 6.58: Pressure contours for case B at $h = 0.234$

presents the comparison of computational Stanton number distribution with the experiment. The best agreement is achieved for $h = 0.234$. This $h$ value corresponds to an impinging shock heating the wall at the geometrical stagnation point. The flow topology corresponds to a type IV interaction. The computation of FLOWer-CNE code [105] suffers from an inadequate grid resolution and predicts a smaller value of the peak heating. The details of the flow field corresponding to $h = 0.1$ and $h = 0.15$ are shown in Figs. 6.55 and 6.56 respectively. The flow topology corresponding to $h = 0.1$ is similar to the type III interaction. The shear layer attachment on the wall is clear in Fig. 6.55 but there is no shock in front of the shear layer attachment. When the impinging shock location is increased to $h = 0.15$, the formation of a well developed supersonic jet takes place but the stagnation streamline does not pass through the center of the jet. When $h$ is increased to 0.234, the flow topology changes to pure type IV interaction as is evident in Fig. 6.57. The stagnation streamline passes through the center of the jet and the jet is normal to the surface. With the aid of Figs. 6.58-6.60, the detailed wave patterns inside the jet can be described. As it was for case A, the supersonic stream inside the jet passes through an embedded shock and expansion fan. As the jet approaches the body, the flow moves upward and downward of the cylinder surface after passing through the detached jet shock and the subsequent subsonic compression. Figures 6.61-6.62 present the experimental and computational interferogram corresponding to $h = 0.234$. The qualitative agreement between the two is quite satisfactory compared to case A. The Schlieren picture as shown in Fig. 6.63 shows the shear layer, the structure of the jet, but it does not provide the information as clear as that was for case A. For cases with thermochemical phenomena, interferograms are more informative. The nonequilibrium nature of the flow fields is shown in the dissociated nitrogen mass fraction contours (Figs. 6.64-6.66). Since the chemical reactions behind a strong shock takes place faster due to low velocity and high
temperature than behind a weak shock, the iso contour plot of the dissociated nitrogen mass fraction is suited to show the triple points and thus the overall jet impingement location. The detailed flow field structure as shown in Figs. 6.55-6.57 is reproduced in the iso plots of the dissociated nitrogen mass fractions. Real gas effects are discussed with reference to type IV interaction corresponding to $h = 0.234$. As shown in Fig. 6.64, there is significant variation in the composition of atomic nitrogen throughout the flow field. The regions showing the highest degree of dissociation are behind the upper bow shock wave where velocity is low and temperature is high. The supersonic jet is essentially frozen because the transmitted oblique shock is considerably weaker than the bow shocks. Even though the temperature behind the detached jet shock is higher than that observed behind the upper bow shock wave, the chemistry has no sufficient time to react due to the high velocity of the flow behind the jet shock in comparison to the velocity behind the upper bow shock wave in the stagnation region.

6.6.4 Case B, shock angle $\beta = 15^\circ$

The shock angle was increased to 15° as proposed by Sanderson and the post-impingement shock conditions were adjusted accordingly by a frozen flow calculation. The computation was performed for $h = 0.268$ which corresponds to the geometrical stagnation point. The initial mesh was the same as it was for the shock angle of 13.2° and the final adapted mesh had 22971 cells. All other flow parameters were identical as for the shock angle of 13.2°. Figures 6.67 and 6.68 present the computational interferogram and Schlieren pictures. The jet shock has become more stronger as compared to the lower impinging shock strength case, as is evident in the Schlieren picture (see Fig. 6.68) as well as the pressure contours (see Fig. 6.71). The flow topology exhibits the type IV interaction pattern. The stagnation streamline passes through the center of the jet and the jet appears to be normal to the
6.6 Flows with shock impingement

Figure 6.61: Experimental interferogram for case B

Figure 6.62: Computational interferogram for case B at $h = 0.234$

Figure 6.63: Computational schlieren picture for case B at $h = 0.234$

Figure 6.64: Iso contours for atomic nitrogen for case B at $h = 0.234$
surface. As before, the wave patterns inside the jet is described completely with the aid of Figs. 6.71-6.73. The increase in peak heating due to increased impinging shock strength is evident in Fig. 6.74. The nonequilibrium nature of the flow field is shown in the atomic nitrogen mass fraction contours in Fig. 6.70. The supersonic jet is nearly frozen and the highest concentration of $N$ atoms is observed behind the upper bow shock wave. There is a significant variation in $N$ composition throughout the flow field.

### 6.6.5 Case C, shock angle $\beta = 14.7^\circ$

This test case represents a high enthalpy condition where significant chemical reactions will take place. Across the weak impinging shock, the composition of the gas does not change and therefore the post-impinging shock conditions have been determined using the frozen flow assumption. As it was for cases A and B, to accelerate the convergence, local time stepping was used on the initial mesh till the essential flow features were properly resolved and then the computations were restarted with global time stepping. The computation on the final mesh was continued till the peak Stanton number and its angular location approached a nearly steady state. The computations were made with different values of $h$ to get a value which corresponds to type IV interaction. Like in the test cases A and B, the initial mesh consists of 3184 cells and the number of cells on the final mesh differs depending on $h$. The final mesh had 16377 and 20775 cells for $h = 0$ and $h = 0.262$ respectively. Figure 6.75 presents the surface Stanton number distributions corresponding to different values of $h$. The comparison of computational Stanton number distributions with the experiment is shown in
6.6 Flows with shock impingement

Figure 6.67: Computational interferogram for case B at $h = 0.268$ ($\beta = 15^\circ$)

Figure 6.68: Computational schlieren picture for case B at $h = 0.268$ ($\beta = 15^\circ$)

Figure 6.69: Details of the flow field for case B at $h = 0.268$ ($\beta = 15^\circ$), sonic line (dots), stream lines (solid)

Figure 6.70: Iso contours for atomic nitrogen for case B at $h = 0.268$ ($\beta = 15^\circ$)
Figure 6.71: Pressure contours for case B at h = 0.268 ($\beta = 15^\circ$)

Figure 6.72: Pressure variation along upper streamline for case B at h = 0.268 ($\beta = 15^\circ$)

Figure 6.73: Pressure variation along lower streamline for case B at h = 0.268 ($\beta = 15^\circ$)

Figure 6.74: Comparison of computed Stanton number distribution at the wall for case B for the two shock angles
6.6 Flows with shock impingement

Fig. 6.76. The flow topology for \( h = 0.262 \) corresponds to a type IV interaction. With regard to the differences in the peak heat flux level and its angular position on the cylinder surface, it is impossible to decide whether the isolated experimental point in the peak region represents the maximum heat flux level or not. On the other hand, away from the jet impingement region, the experimental and numerical data are in very good agreement. As evident in Fig. 6.77, the formation of a supersonic jet takes place only for \( h = 0.2 \) and \( h = 0.262 \). As the value of \( h \) is increased from \( h = 0 \) to \( h = 0.35 \), the flow topology changes significantly as shown in Figs. 6.83-6.87. For \( h = 0.2 \), though the formation of a well developed supersonic jet takes place, the stagnation streamline does not pass through the center of the jet. The jet is inclined to the cylinder surface (see Fig. 6.78). On the other hand, in the case of \( h = 0.262 \), the jet appears normal to the surface and the stagnation streamline passes through the center of the jet (see Fig. 6.79). Even though the jet is broader and the detached jet shock is nearer to the cylinder surface for the flow corresponding to \( h = 0.2 \) as compared to \( h = 0.262 \), the peak heating is more enhanced for \( h = 0.262 \) than for \( h = 0.2 \). This happens because the flow topology for \( h = 0.262 \) exhibits the pure type IV interaction, where the jet stream hits the surface normally, whereas for \( h = 0.2 \), most of the particles in the jet stream sweeps along the surface of the cylinder downwards. The detailed wave patterns inside the jet corresponding to the flow topology for the case \( h = 0.262 \) can be described with the aid of Figs. 6.80-6.82. The supersonic stream inside the jet passes through an embedded shock and expansion fan. As the jet approaches the body, the flow moves upward and downward of the cylinder surface after passing through the detached jet shock and the subsequent subsonic compression. The extent of the subsonic compression subsequently after the jet shock compression is either absent or of smaller magnitude.

Figures 6.89 and 6.90 present the computational interferograms corresponding to \( h = 0.2 \) and \( h = 0.262 \) respectively. The qualitative agreement between the experimental and computational interferograms is better for this case than for cases A and B. The nonequilibrium nature of the flow fields is shown in the dissociated nitrogen mass fraction contours in Figs. 6.83-6.87. Real gas effects are discussed with reference to type IV interaction, corresponding to \( h = 0.262 \). As shown in Fig. 6.86, there is significant variation in \( N \) composition throughout the flow field. The regions showing the highest degree of dissociation is behind the upper bow shock wave. The dissociation level is significantly high in this case compared to case B. The significant dissociation takes place just behind the jet shock as compared to case B.

With the aid of Figs. 6.91-6.94, the advantage of the grid adaptation compared to an uniform grid is described. Two uniform meshes with number of cells 19600 and 32400 respectively were used for the computation of this test case. Figures 6.91 and 6.92 show the zoomed view of the uniform mesh with 32400 cells and the adapted mesh with 20775 cells respectively. The supersonic jet in case of the adapted grid is more broader and extends closer to the surface before it becomes subsonic, than in the case of the uniform meshes as shown in Fig. 6.93. The peak heating level is also more intense for the adapted grid (Fig. 6.94). The adapted grid which has around 12000 cells fewer
than the uniform mesh captures the relevant phenomena more robustly. Thus the grid adaptation is always advantageous to be used to simulate complex flow fields where the prior knowledge of the different flow patterns is difficult to analyse, like in the present case. However the stanton number profiles of uniform meshes are nearly smooth unlike the adaptive mesh, where wiggles are present away from the peak heating region.
6.6 Flows with shock impingement

Figure 6.79: Details of the flow field for case C at h = 0.262, sonic line (dots), stream lines (solid)

Figure 6.80: Pressure contours for case C at h = 0.262

Figure 6.81: Pressure variation along upper streamline for case C at h = 0.262

Figure 6.82: Pressure variation along lower streamline for case C at h = 0.262
Figure 6.83: Iso contours for atomic nitrogen for case C at h = 0

Figure 6.84: Iso contours for atomic nitrogen for case C at h = 0.1

Figure 6.85: Iso contours for atomic nitrogen for case C at h = 0.2

Figure 6.86: Iso contours for atomic nitrogen for case C at h = 0.262
6.6 Flows with shock impingement

Figure 6.87: Iso contours for atomic nitrogen for case C at h = 0.35

Figure 6.88: Experimental interferogram for case C

Figure 6.89: Computational interferogram for case C at h = 0.2

Figure 6.90: Computational interferogram for case C at h = 0.262
Figure 6.91: Uniform grid (no. of cells = 32400) for case C at $h = 0.262$

Figure 6.92: Zoomed view of final adapted mesh (no. of cells = 20775) for case C at $h = 0.262$

Figure 6.93: Comparison of jet shape for adapted and nonadapted grids for case C at $h = 0.262$, geometry of sonic lines

Figure 6.94: Comparison of Stanton number distribution at the wall for adapted and nonadapted grids for case C at $h = 0.262$
6.6.6 Case C, shock angle $\beta = 16^\circ$

The shock angle was increased to $16^\circ$ and the post-impingement shock conditions were adjusted accordingly by a frozen flow calculation. The computation was performed for $h = 0.29$ which corresponds to the geometrical stagnation point. The initial mesh was the same as it was for the case of shock angle of $14.7^\circ$ and the final adapted mesh had 28276 cells. All other flow parameters were the same as for shock angle of $14.7^\circ$. The computations were carried out till the jet impingement location converged to a steady value. The jet unsteadiness was observed but of small significance. Figures 6.95 and 6.96 present the computational interferogram and the detailed flow field. With the increase in shock strength, vortices are formed due to high velocity gradients across the shear layer. There was no pattern of vortex formation and shedding found in this case. The jet shock has become more stronger as compared to the lower impinging shock strength case. The flow topology exhibits the type IV interaction pattern. The stagnation streamline passes through the center of the jet and the jet appears to be normal to the surface. The peak heating enhancement has increased with the increment in the shock angle, as is evident in Fig. 6.98. The nonequilibrium nature of the flow field is shown in the atomic nitrogen mass fraction contours in Fig. 6.97. The supersonic jet is nearly frozen and the highest concentration of $N$ atoms is observed behind the upper bow shock wave. The high concentration of the $N$ atoms is also observed just behind the jet shock. There is a significant variation in $N$ composition throughout the flow field.

6.7 Summary of the results

The present computations could well resolve the complex features of the flow phenomena associated with the type IV shock interaction. The differences between computed and experimental results may be caused by the uncertainties of the geometrical parameters of the impinging shock, variations in free stream conditions, spanwise variation of the impinging shock location etc. The type IV interaction flow field is strongly sensitive to the shock impingement location. Interferometric comparisons are hindered even in the case of flows without shock interaction due to the 3d effects of the flow field. Particularly experimental interferogram of case A is severely affected by non-uniform free stream conditions and 3d effects of the flow field. A general impression that arises from the present comparison between computational and experimental Stanton number distributions is that, for an Edney type IV interaction, the very narrow physical width of the peak heat transfer calls for high accuracy both in the numerical simulation and in the experimental measurements. Thus, on one hand, a proper grid refining is necessary for the numerical simulations, on the other hand, an adequate refinement level should also be mandatory for the experimental measurements, both in terms of spacing and of the dimension of the gauges. In the present study, the grid refinement is adequately done by the adaptation strategy. Considering the possibilities of so many parameters affecting the flow field during experiment, the comparison between the present computational results and experiment is quite satisfactory. Figure 6.99 presents the Stanton number distributions representing a type IV
Figure 6.95: Computational interferogram for case C at $h = 0.29 \ (\beta = 16^\circ)$

Figure 6.96: Details of the flow field for case C at $h = 0.29 \ (\beta = 16^\circ)$, sonic line (dots), stream lines (solid)

Figure 6.97: Iso contours for atomic nitrogen for case C at $h = 0.29 \ (\beta = 16^\circ)$

Figure 6.98: Comparison of computed Stanton number distribution at the wall for case C for the two shock angles
6.7 Summary of the results

The comparison of peak heating level between cases A and C shows that the peak heat transfer intensification decreases with the increase in stagnation enthalpy. The peak heating intensification for case B and case C is nearly the same. Thus, the computational results appear to confirm the experimental conclusions that the real gas effects decrease peak heating intensification, which is in contrast to the variable $\gamma$ model of Edney, where real gas effects are suggested to significantly increase the peak pressure with decreasing ratio of specific heats. The Stanton number profiles are expected to change quantitatively in the same way with the consideration of some important parameters like wall catalycity, turbulence, further grid refinement, small variations in $h$, impinging shock boundary conditions, etc. However, the qualitative aspect of the comparison will remain unchanged. Further, care must be taken to interpret this trend since the results are presented in terms of dimensionless form. The dimensional heat transfer increases considerably with the stagnation enthalpy. Furumoto et al. [29] arrived at the same conclusion as in the present work. The reduction in heat transfer enhancement due to real gas effects is also found by the analytical treatment of the problem by Sanderson [88], [89].
Chapter 7

Conclusion

In the framework of the work presented in this thesis, the adaptive CFD code QUADFLOW has been successfully extended to take into account real gas effects. In its basic form, the flow solver assumes a thermally and calorically perfect gas model. The present work assumes a five component air model, consisting of the species $N_2$, $O_2$, $NO$, $N$ and $O$. The governing equations were augmented by the species mass conservation equations and the vibrational energy conservation equations for molecular components. Various models for chemical reaction rates and the energy exchange processes were implemented. Different flux vector and flux splitting methods were integrated in the code. The extended version of the code was used to run some typical reactive and non reactive test cases. The agreement between the computed results and the available experimental, theoretical and computational results were excellent.

The rate at which the relaxation processes occur behind strong shock waves has an important effect on the flow field around high-speed missiles and re-entering vehicles. The study of relaxation processes behind a normal shock wave is an excellent numerical test case to investigate the influence of different physiochemical modelling on the overall flow field. In this regard, the stationary, inviscid one dimensional flow of a five component air in thermal and chemical nonequilibrium behind a normal shock was investigated. The essential features of the relaxation process were discussed through the numerically calculated distribution of the flow variables for different free stream velocities. It was observed that different reaction rate models have significant influence on the relaxation processes. The reaction rate models differ considerably at high temperatures, which result in different relaxation length. Similar influences are observed with models of energy exchange processes. A comparison was made between a four temperature and two temperature model. Considering the uncertainties associated with the modelling of different energy exchange processes, it was observed that, it may not be worthwhile to introduce more and more temperatures in CFD calculation. The introduction of more and more temperatures even brings back the problem of numerical stiffness.

Further, a similar study was made using a two dimensional nitrogen flow over a cylinder. For this test case, experimental results are available from Hornung. Parametric sensitivity studies carried out in the present work using the chemical kinetic models and relaxation models show that a practical
quantity like the shock stand-off distance may change by as much as \(30\%\) between the extreme cases. From the computed flow field, interferograms were constructed and compared with the experimental interferogram. It was observed that though for different chemical kinetic models, the shock stand-off distance may agree well with the experimental one, but the relaxation process may vary widely. Thus the shock stand-off distance is not a sufficient parameter to validate the physiochemical modelling. The judgment regarding the correctness of one model over another model which have been used in this work, is not justified considering the uncertainties associated with the different models. By selecting a proper set of models, experimentally obtained flow fields can be reproduced within a good accuracy using a numerical simulation.

A series of numerical computations were carried out to investigate the real gas effects on the shock-shock interaction phenomena. The present study mainly concentrated on type IV interference pattern. Three different test conditions were used for the computations. Experimental results for all these cases were available from Sanderson. The first case, A, represents a low enthalpy control condition where the only real gas effects are a partial excitation of the vibrational modes in the stagnation regions of the flow. Case C represents a high enthalpy condition that was chosen to highlight the influence of nonequilibrium thermochemistry on the problem. Case B is an intermediate enthalpy condition that was designed to aid interpretation of the differences in the flow mechanisms for cases A and C. Thus by choosing three different test cases, representative of different regimes of hypervelocity flow, it was convenient to arrive at a conclusion regarding the influence of real gas effects on peak heat transfer enhancement. The present computations could resolve the complex features of the flow phenomena associated with the type IV shock-shock interactions. Considering the complex nature of the flow field and the influences of various parameters on it, the comparison between the present computational results with experimental one is quite satisfactory. The computational results appear to confirm the experimental conclusions that the real gas effects decrease peak heating intensification.
Bibliography


## Appendix A

### Reaction rate models

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<td>4.60E11</td>
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<td>75500</td>
<td>7.95E17</td>
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<tr>
<td>( NO + O \rightarrow 2N + O )</td>
<td>4.60E11</td>
<td>-0.50</td>
<td>75500</td>
<td>7.95E17</td>
<td>-2.00</td>
<td>75500</td>
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<td>( NO + O_2 \rightarrow 2N + O_2 )</td>
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<td>7.95E17</td>
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Table A.1: Forward rate constants for Park (85) and Park (87) model in S.I. units
<table>
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<th>Park (90)</th>
<th>Dunn and Kang</th>
</tr>
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<td>$C_i r$</td>
<td>$n_i r$ $E_i r/k$</td>
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<td>-1.50 59500</td>
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<tr>
<td>$O_2 + O_2 \rightarrow 2N + O_2$</td>
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<td>-1.50 59500</td>
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<tr>
<td>$NO + N \rightarrow 2N + N$</td>
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Table A.2: Forward rate constants for Park (90), and Dunn and Kang model in S.I. units.
## Reaction rate models

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Gupta</th>
<th>Curve fit</th>
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<td>( \text{N}_2 + N \rightarrow 2N + N )</td>
<td>( C_{tg} )</td>
<td>( n_{tg} )</td>
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Table A.3: Forward rate constants for Gupta, and Curve-fit model in S.I. units
Appendix B

Constants used in the physico-chemical modelling

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<th>Component</th>
<th>$M_0$ [kg/mol]</th>
<th>$R_0$ [J/kg/K]</th>
<th>$d_0$ [m]</th>
<th>$d_0^{(0)}$ [K]</th>
<th>$d_0^{(1)}$ [K]</th>
<th>$d_0^{(2)}$ [K]</th>
<th>$\delta_i$ [K]</th>
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Table B.1: Thermodynamic constants, taken from Ref. [55]
Table B.2: Coefficients used in the computation of vibrational relaxation time in eq. (2.82) [55]

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<th>$C_{0mi}$</th>
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Table B.3: Viscosity coefficients for Blottner Model

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Appendix C

Computational interferograms

Optical flow visualisation is an important tool for understanding the complex flow phenomena in aerodynamics. For the high temperature flow, reliable and well known techniques, which also offer the possibility of obtaining quantitative results, have to be used. The Shadowgraph or Schlieren techniques for the flow visualisation are not the suitable methods for the quantitative measurements of the fluid density. These methods are suitable for obtaining a quick survey of flow fields with varying density, particularly shock waves and temperature boundary layer [55], [70]. However these methods can not resolve the density changes in the relaxation zone, in case of a chemically reactive flow field, because of the weak density gradients. With an interferometer, information about flow structures such as bow shock waves and shear layers around a model can be made visible and flow densities can be obtained. That is the reason why it is widely used in the area of high speed flow research [53].

The Mach-Zehnder interferograms are created by interfering two beams: the reference beam and the object beam. The reference beam does not pass through the flow field and its phase is not changed. The object beam does pass through the flow field, and its phase is changed by the density variations. When the object beam interferes with the reference beam, under the assumption that the conditions of optical coherence are fulfilled, they constructively and destructively combine to form a manifest series of dark and light fringes [115]. In case of a finite fringe interferogram, the phase shift of the object beam relative to the reference beam is obtained by integrating the following equation along a line of sight [89], [115]:

\[
\phi = \frac{2\pi}{\lambda} \int_{a}^{l} (n - n_0) dl
\]  

(C.1)

The fringe shift is given by

\[
\Delta N = \frac{1}{2} \int_{a}^{l} (n - n_0) dl
\]  

(C.2)

For reacting gases, the refractive index \( n \) is given by [70]

\[
n = 1 + K \rho,
\]

(C.3)

where the Gladstone-Dale constant \( K \) is given by

\[
K = \sum_{\alpha} K_{\alpha} X_{\alpha}
\]  

(C.4)
The values of Gladstone-Dale constants, $K_\alpha$, are given in Table C.1. Assuming two-dimensional flow, the integration is simplified by multiplying only with the spanwise length $l$ of the model. The intensity, $I$, of the interference of the recombined beams is related to the phase shift by

$$I = \cos^2(\phi/2)$$

(B.5)

Because of the varying concentration of the species in the flow and the different Gladstone-Dale coefficient of the several species, a conversion of the measured interferogram into a density field is hardly possible. So, for the comparative studies of the flow field, it is much easier to produce an interferogram out of the data of the numerical simulation. In the numerical interferograms, the areas between the lines of constant fringe shift in the field are alternately filled black and white. The values for the isolines has to be chosen so that for a fringe shift difference of one, a white and a black fringe occur.

<table>
<thead>
<tr>
<th>Species</th>
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<tbody>
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<td>$O$</td>
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Table C.1: Gladstone-Dale constants, Sources: [55], [70], [115]
Resume

Personal Details
Name Sanjeev Kumar
Date of Birth 03.01.1973
Place of Birth Motihari, Bihar (India)
Family status Married

Education
1988 Matriculation (10th), B.S.E.B., Patna, Bihar
1990 Intermediate (10 + 2), B.I.E.C., Patna, Bihar
04/1996 B.E.(Eq.), The Aeronautical society of India, New Delhi
03/1999 M.Tech., Indian Institute of Technology, Madras

Professional experience
11/1996 - 07/1997 Engineer (Contract), CEMILAC, DRDO, Bangalore
06/1999 - 06/2001 Research associate, Graduate study programme “Transport processes in hypersonic flow”, Aachen University
07/2001 - 03/2004 Research scholar, Shock Wave Laboratory, Aachen University
since 04/2004 Research scholar, Laboratory of Mechanics, Aachen University

Academic excellence
1996 All India Rank 14 in Graduate Aptitude Test in Engineering (GATE)
1998 Selected as DAAD scholar for M.Tech. thesis work at Shock Wave Laboratory, Aachen University