Abstract

SALAZAR, GIOVANNI. High Fidelity Modeling of Re-entry Flows Using a Hybrid LES/RANS Approach. (Under the direction of Dr. Jack R. Edwards.)

The performance of a hybrid Large-Eddy Simulation/Reynolds-Averaged Navier-Stokes (LES/RANS) turbulence model is evaluated for hypersonic base flow problems using North Carolina State University’s REACTMB in-house code. The method is validated with data obtained from the CUBRC LENS facility at different Reynolds numbers for a Mach 6 flow around a spherical capsule. Pressure and heat transfer comparisons are made with the experiment for a high Reynolds number (fully turbulent) test case, and for a lower (nominally transitional) Reynolds number. Additionally, LES/RANS results are compared with Detached Eddy Simulation (DES) and Reynolds-Averaged Navier-Stokes (RANS) predictions. The LES/RANS and DES results are in very good agreement with each other and the experimental data, whereas the RANS model tends to overpredict heat transfer in the separated region. Different numerical aspects of the LES/RANS methodology and the computational approach are also evaluated, such as blending between LES and RANS, filtering experimental time traces, and time-averaging CFD results. The implementation of thermal nonequilibrium capabilities to REACTMB is also described in detail. A code-to-code verification study with NASA’s DPLR code shows excellent agreement between the two, therefore confirming the correct implementation of the thermal and chemical models. Finally, three-dimensional simulations are presented for a Mach 16 flow around a flight-scale spherical capsule at conditions obtained from the Fire II flight test. The results showcase the integration of thermochemical nonequilibrium capabilities with the LES/RANS model in REACTMB for a more realistic re-entry problem.
High Fidelity Modeling of Re-entry Flows Using a Hybrid LES/RANS Approach

by
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Dedication

This work is dedicated to my wife, my parents and my sister for their love, support and understanding.
Biography

The author was born in San Jose, Costa Rica in November of 1987, and grew up in the town of San Rafael, Heredia. After moving with his family to the United States in 2000, they settled in the city of Concord, North Carolina. Upon completion of high school at J.M. Robinson High School in Concord, Salazar was awarded the Gates Millennium Scholarship. He attended Embry-Riddle Aeronautical University in Daytona Beach, Florida for a year, and later transferred to North Carolina State University to pursue a degree in aerospace engineering. While at NC State, Giovanni was first introduced to computational fluid dynamics (CFD) in a course offered by Dr. Jack Edwards, which became one of his main interests during his undergraduate years. Additional research experience under Dr. Hong Luo during his senior year solidified his interests in CFD and numerical methods. In 2011, Salazar graduated from NC State University with a Bachelor of Science in aerospace engineering, a minor in mathematics, a minor in physics, and class valedictorian honors. He continued his studies at NC State to pursue a Master of Science in aerospace engineering under the direction of Dr. Edwards, where he focused on applications of LES/RANS turbulence models for simulating hypersonic base flows. During his Master’s career, Salazar was admitted into NASA’s Graduate Co-op program at Lyndon B. Johnson Space Center (JSC). While at JSC, he worked with the aerothermodynamics group in the Aeroscience and CFD branch, where he will join as a full-time employee upon completion of his graduate degree.

Outside of school and research, Giovanni enjoys spending time with his wife, family and friends, playing and watching soccer, and exercising.
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Nomenclature

Roman Letters

\( a \)  
\( a \) sound speed

\( A_{1r} - A_{5r} \)  
constants for equilibrium constant curve fit

\( C_M \)  
LES model constant

\( C_p \)  
specific heat at constant pressure

\( C_v \)  
specific heat at constant volume

\( C_f \)  
constant for forward reaction rate constant

\( \text{DAM} \)  
Danköhler number

\( e \)  
internal energy per unit mass

\( E \)  
total energy per unit mass

\( E_{a,r} \)  
activation energy for reaction \( r \)

\( \vec{E}, \vec{F}, \vec{G} \)  
sum of inviscid and viscous flux vectors in \( x,y,z \) direction

\( F \)  
vector of inviscid fluxes

\( f^{\text{Ducros}} \)  
Ducros function

\( G \)  
vector of viscous fluxes

\( h \)  
specific enthalpy

\( H \)  
total enthalpy per unit mass

\( k \)  
thermal conductivity; turbulent kinetic energy

\( K_{eq} \)  
equilibrium constant

\( k_f, k_b \)  
forward, backward reaction rate constants

\( l_{\text{inn}}, l_{\text{out}} \)  
inner, outer boundary layer length scale

\( M_n \)  
species molecular weight

\( n \)  
normal vector

\( P \)  
pressure

\( P_r \)  
Prandtl number

\( q \)  
heat flux vector

\( q_w \)  
wall heat flux

\( q_L \)  
laminar heat flux

\( q_T \)  
turbulent heat flux

\( R \)  
steady residual

\( R_n \)  
species gas constant

\( R_u \)  
universal gas constant

\( Re_D \)  
Reynolds number based on capsule diameter

\( RR \)  
reaction rate
S  vorticity vector
Sc  Schmidt number
t  time
T  temperature
Tₜ  effective temperature for computing forward reaction rate constant
TB  third body efficiency factor
t₁₂, t₃₄  stress tensor
tr  characteristic flow residence time
tₕ  characteristic time scale of chemical reactions
tₔ  characteristic time scale of chemical reactions
u, v, w  velocity components in the x,y,z directions
U  vector of conserved variables
ui  instantaneous velocity
Uᵢ  mean velocity
V  vector of primitive variables
Vnᵢ  diffusion velocity of species n in i coordinate direction
W  source term vector
x₁, x₂, x₃  index notation for x,y,z directions
Yₙ  mass fraction of species n

Greek Letters

δ₁₂  kronecker delta
Δ  LES filter width
κ  von Kármán constant
ρ  density
νₜ  turbulent kinematic eddy viscosity
νₜ,SGS  subgrid scale turbulent kinematic eddy viscosity
ν', ν''  stoichiometric coefficients
ε  turbulent kinetic energy dissipation rate
μ  laminar molecular viscosity
μₜ  turbulent viscosity
τ  vibrational relaxation time
τ₁₂  Reynolds stress tensor
τ₁₂,SGS  subgrid scale stress tensor
θₜ  characteristic temperature of vibration
ω  turbulence frequency
λ  ratio of boundary layer length scales
Γ  LES/RANS blending function
\dot{\omega}_n  production rate of species n
\dot{\omega}_v  vibrational energy production rate
\dot{\omega}_{tr-v}  vibrational energy production due to energy exchange between trans/rot and vibrational modes
\dot{\omega}_{v,spec}  vibrational energy production due to creation of molecules
Ω  cell volume

**Superscripts**

trans  translational energy mode
rot  rotational energy mode
vib  vibrational energy mode
elec  electronic energy mode
tr  translational/rotational
SGS  subgrid scale term
c  convective component
p  pressure component
n  time level

**Subscripts**

r  rotational mode
v  vibrational mode
e  electronic mode
i,j,k  cell indices, spatial coordinates
T  turbulent quantity
∞  freestream
n  species
L,R  left and right states
**Accents**

- vector
- time-averaged quantity
- density-averaged quantity
- time-fluctuation
- mass-fluctuation
- resolved scale term

**Abbreviations/Acronyms**

- BSL: Baseline
- CFD: Computational Fluid Dynamics
- CHAR: Charring Ablator Response
- DES: Detached Eddy Simulation
- DNS: Direct Numerical Simulation
- DPLR: Data Parallel Line Relaxation
- ILU: Incomplete Lower/Upper
- LDFSS: Low-Diffusion Flux-Splitting Scheme
- LDPPM: Low-Dissipation PPM
- LES: Large Eddy Simulation
- MPCV: Multi-Purpose Crew Vehicle
- MSL: Mars Science Laboratory
- NRMS: Normalized Root Mean Square
- PPM: Piecewise Parabolic Method
- RANS: Reynolds-Averaged Navier Stokes
- RCS: Reaction Control System
- SA: Spalart-Allmaras
- SGS: Subgrid Scale
- SST: Shear Stress Transport
- TPS: Thermal Protection System
- TVD: Total Variation Diminishing
Chapter 1

Introduction

Even though there is no concrete definition of where the hypersonic flight regime begins, in general, hypersonic flows are defined by Park [50] as flows “in which the square of Mach number is much greater than unity”. The first hypersonic flight dates all the way back to 1949 [4], yet it still remains a relatively unexplored regime which presents many unique challenges to today’s aerospace engineers. Some flow phenomena common to hypersonic flows include thick boundary layers, strong shocks, thin shock layers, rarefied gases and real gas effects. One particular problem, which has been of great interest to aerothermodynamicists for decades, are re-entry type flows, where the aerodynamic heating loads must be determined from predictions of the environment, and all of the aforementioned phenomena (in addition to turbulence and transition) must be taken into account. In order to cope with the high levels of heating, blunt bodies are used for atmospheric entry, where the idea is to have the large shock layer absorb a great portion of the energy which would otherwise be deposited onto the vehicle’s surface. These hypersonic wake flows have been investigated experimentally and theoretically since the 1950’s [33], and considerable experience has been gained from previous programs such as the Apollo [51] and Space Shuttle programs, and many of the interplanetary probes. Those spacecraft, in particular those from the Apollo and Space Shuttle programs, were designed by use of engineering correlations (such as Fay-Ridell and Modified Newtonian Theory) and experimental testing [7]. Today, with large advances in numerical methods and computational power, computational fluid dynamics (CFD) has become an essential tool for research and design. Thanks to CFD, design cycles of vehicles have reduced significantly, and the rapid spread of computational efforts can be (in part) attributed to more robust codes, lower computational costs and better grid generation software [42].

As NASA looks to send missions beyond low Earth orbit once again, recent efforts for the Mars Science Laboratory (MSL) and the Orion Multi-Purpose Crew Vehicle (MPCV) have highlighted difficulties in modeling separated wake flows. Even with the available computational
tools, Wright [66] estimates that uncertainty levels for design of environments on the afterbody of re-entry vehicles is approximately 200-300%, which results in large safety margins in thermal protection system (TPS) design and, ultimately, increases in mass. Therefore, numerical simulations of such flows still present a great challenge to engineers.

1.1 Literature Survey

Significant efforts have been focused on the prediction of heat transfer in complex hypersonic flows by a combination of experimental programs and computations. One of the most significant collaborative efforts between scientists from United States and Western Europe, took place in the 1990’s through the fluid dynamics panel of the Advisory Group for Aerospace Research and Development (AGARD). By collecting data from different facilities across the world, and carrying out independent code testing, the effort was focused on investigating hypersonic capabilities and needs of the time [1]. Using data obtained on a 70° sphere-cone model representative of a re-entry vehicle, much insight was gained on forebody and afterbody heating predictive capabilities. Hollis and Perkins [29] showed that laminar forebody heating levels could be predicted with very good accuracy using computational methods, but that the inability to precisely predict how the shear layer reattached on the sting resulted in much greater differences between predictions and experiment for afterbody heat transfer. Other similar studies showed that the resulting heat flux when the shear layer is transitional is greater than a fully turbulent shear layer, and could result in localized heating values which are 40-75% of the stagnation heating [33] [47] [34]. Previous research has also focused on studying the stagnation point heating during re-entry. It has been shown that it is sensitive to the atmospheric composition, freestream disturbances, roughness and particle effects [32] [35]. Additional interactions which complicate wake flow problems include impingement of RCS jet plumes [13], localized regions of rarefied gas [34], radiative heating on the afterbody due to a hot wake neck region [27], lack of flight and ground data for code validation [13], material properties uncertainties [30], and transition and turbulence modeling.

Transition remains, as Bertin [7] points out, a “known unknown” during our design process. In 1998, as part of the post flight analysis of the European ARD, researchers found that they had underpredicted heating levels during some portions of re-entry due to their inability to model the transitional regime [62]. During the design of the MSL, only empirical correlations were available as a best estimate for transition, and the vehicle still had to be designed assuming fully turbulent environments during the entire trajectory [13]. In addition to natural transition mechanisms, roughness induced transition must also be considered during re-entry problems. Schneider [54] presents an extensive review of previous investigations of roughness transition which date back to the 1950’s, and he describes the complex dependence on geometry, roughness sizes, Mach
number, Reynolds number, wall temperature, tunnel noise (in ground tests) and angle of attack. More recent works by Amar et al. [2] and Hollis [31] address heating augmentations on models of the Orion MPCV forebody due to boundary layer tripping by the presence of protuberances and cavities.

Despite the many difficulties with transition prediction, computational models for fully laminar and fully turbulent flows have been developed and implemented on bluff body problems for decades. It has been found, in general, that current numerical methods allow us to predict laminar wake flows with very good accuracy. In an extensive study using conditions and data from the AS-202 flight, Wright found that current laminar predictions (using correct assumptions) are accurate to within 20% of the experimental data, which was determined to be within the uncertainty of the flight instrumentation [67]. Edquist et al. also claim that computational predictions can be made to within 25% uncertainty for laminar environments [13]. Unfortunately, turbulence modeling approaches have still not reached such level of predictive capabilities for separated flows, and as Longo points out, turbulence remains one of the “oldest unresolved fluid dynamics problems” [42]. Currently, engineering practices rely mostly on Reynolds Averaged Navier Stokes (RANS) methods for modeling turbulent flows. These methods model the time-averaged properties of the flow and determine the effects of turbulence on the mean velocity by modeling an effective Reynolds stress. RANS simulations are the simplest and least expensive ways to model turbulence, but they lack the ability to accurately simulate unsteady separated wake flows [5]. Using the Spalart-Allmaras (SA) and k-ω RANS models, Forsythe, Hoffmann and Dietiker modeled Herrin and Dutton’s Mach 2.46 supersonic base experiment using unstructured grids in an attempt to replicate the size and shape of the recirculation region, the shear layer separation, and flow properties in the base region. It was determined that both RANS models underpredict the separation bubble and they underpredict the base pressures by up to 80%. However, the SA model showed much higher dissipation levels than the two equation model [19]. In a similar study, Forsythe, Hoffmann, Cummings and Squires compared the SA model to Menter’s SST on different structured and unstructured grids, and found that both models fail to resolve the unsteady flow field features and Mach number distributions. The results showed some improvement when using compressibility corrections with the RANS models, however, they introduced unrealistic radial variation in the base pressures, where the experiment saw approximately constant values due to enhanced turbulent mixing [20]. In attached regions, RANS models yield good results (in general) if the flow is fully turbulent, and they tend to overpredict heat flux if the flow is transitioning to turbulence. Therefore, RANS models have been found to be conservative for design purposes on attached flows. However, using an algebraic model to study the heating on a model of the MSL at an angle of attack, Edquist et al. [13] found that computations using an algebraic turbulence model underpredicted heating levels on the forebody leeside by up to 15% when compared to data obtained from different
hypersonic test facilities. Using a RANS approach to model the Fire II flight experiment, Sinha found that the predicted size of the recirculation region was too small which resulted in low base pressures and very high temperatures in the base [56]. In an effort to validate the most advanced and popular RANS models of the time, Brown [9] compared different RANS models (and corrections) by applying them to different hypersonic flows such as flat plates, compression corners, the 70° sphere-cone model and the Ames all-body experiment. After looking at two variants of the Wilcox k-ω models, Menter’s SST model, the Baldwin-Lomax algebraic model, and the Spalart-Allmaras model, Brown concluded that all models provide very good results for attached flows, in particular the SST approach, but they all showed great discrepancies in detached flows. The study also highlights how each model performs differently depending on the problem being solved, and therefore there is not one “better” RANS model for all problems and flow conditions. Examples of more advanced RANS models (or sometimes known as “second generation RANS models”) have also been found in the literature. Even though these methods are relatively easy to implement on existing solvers with RANS models, they are still in great need of validation, but initial studies show good improvements over the typical RANS methods [21] [52].

The difficulties found when modeling separated flows with RANS models are not surprising, since these models were developed by “calibrating” with wall bounded flows, which are fundamentally different from separated wake flows. Travin et al. [63] explain that Reynolds averaging eddies found in the wake region, which are different from the “standard eddies” found in shear layers (used to calibrate RANS models), results in great discrepancies for separated flows. For this reason, higher fidelity models will be the “basis of turbulence prediction for a large class of flows”.

In contrast to RANS, Direct Numerical Simulation (DNS) techniques are able to resolve all scales present in a turbulent flow, but DNS applications of practical flows are currently too computationally expensive. Another approach, which is also able to resolve unsteady features of a flow, is Large Eddy Simulation (LES) which was introduced in the 1960’s by Smagorinsky [41]. LES works by resolving the larger turbulence structures and modeling the effects of subgrid scales. Although not as computationally expensive as DNS, an LES model has very severe spacing requirements near walls, which has led to the development of hybrid models by coupling LES with RANS models. Therefore, hybrid LES/RANS approaches resolve the largest scales of turbulence using LES, while modeling the smaller near-wall scales using the desired RANS model.

Hybrid LES/RANS approaches have shown significant improvements over conventional RANS models in supersonic separated flows. During the last decade or so, several studies using Detached Eddy Simulation (DES) have shown promising results when modeling supersonic and hypersonic bluff body flows [60]. DES is a type of hybrid LES/RANS model which uses a single
turbulence model as a subgrid-scale model in regions where the grid spacing is fine enough for LES, and as a RANS model inside boundary layers. Forsythe, Hoffmann and Dietiker [19] modeled Herrin and Dutton’s supersonic base experiment using DES with an unstructured solver and were able to predict pressure coefficients which were within 9% of the experiment, in contrast to RANS predictions which were on the order of 20%. They were also able to match the peak turbulent kinetic energy ($k$) values and Reynolds stresses to the experiment. Forsythe, Hoffman, Cummings and Squires [20] found that their DES results obtained using the coarsest grid for Herrin and Dutton’s problem produced results very similar to RANS on a fine grid. Their DES results gave a very good comparison to the experiment, and it was found that DES was not particularly sensitive to the RANS model selected nor to the implementation of compressibility corrections. Kawai and Fuji [36] also modeled the same experiment using a different LES/RANS approach. Their approach involved using the Baldwin Lomax RANS model near walls and a Smagorinsky SGS model in LES mode, using a blending function which depended explicitly on grid spacing to transition. Their results showed that the model is able to predict a shear layer similar to the experiment, unlike RANS results, which significantly alter the shape of the shear layer due to high eddy viscosity levels in the base region. Despite the good results obtained using DES, reports of the so-called modeled stress depletion (MSD) observed in several studies led to the development of a corrected version of DES known as Delayed DES (DDES). This improvement introduced by Spalart et al. [59] prevents the model from switching to LES mode near walls where the wall-parallel grid spacing is less than the thickness of the boundary layer, and ensures that the entire boundary layer is treated in RANS mode, as it was originally intended with DES. This improvement is particularly important in hypersonic problems where thick boundary layers are present. In a grid sensitivity study using DES at a transitional Reynolds number, Sinha [58] found that grid independence could not be achieved. As the grid was refined, the eddy viscosity levels kept decreasing which led to more resolved flow structures, resulting in changes in heat flux and pressures for each grid case. Travin et al. [63] also point out the big challenge of designing a grid for LES and hybrid methods, where a more refined grid does not always yield more accurate results (as compared to experiment). In a similar sensitivity study of Reynolds number, Sinha [56] found that when modeling the Fire II flight experiment, the separation bubble size was not very sensitive to a one order of magnitude change in density, however, the heating levels on the backshell saw significant variation.

Using data obtained from the Reentry-F Flight Experiment, the results of Barnhardt and Candler [6] show much improvement over RANS models when using a DES approach with a five species air model by Park [50]. In addition, their study highlights the sensitivity of computational results to uncertainties in the flight data, where a small change in the vehicle’s orientation resulted in large discrepancies between the flight and CFD. More recently, Barnhardt, Candler and MacLean presented a new set of data for CFD validation and they obtained very good
results when considering a representative model of the Orion MPCV at a Mach number of 6 using the DES methodology, and significant improvements over two different RANS models (SST and SA) were shown. Even in unsteady computations, RANS models were not able to resolve the temporal evolution of the flow and significantly overpredicted heat flux levels on the afterbody of the vehicle. As a result, the integrated relative error for the heat transfer gauges located in the wake was shown to be 1.5 times greater with RANS than with DES [5].

1.2 Motivation

As an alternative to DES, many other different LES/RANS approaches have also been developed recently. Fröhlich [21] presents a very good introduction and review of the different hybrid models in the literature, and in the end, the differences between methods lie mostly on how the transition from RANS to LES is achieved. Coming up with an appropriate continuous blending technique remains a topic of research in the CFD community. Additionally, each hybrid model presents different issues and sensitivities depending on the problem being modeled, which highlights the importance of testing and validating each approach to find out its advantages and limitations. The hybrid LES/RANS approach developed at North Carolina State University has been used extensively to study internal flows for scramjets, supersonic flow over flat plates and compression corners, and shock-boundary layer interactions ([14][22][23][18][70][16][15]). However, these methods have not been previously validated for re-entry type problems. Therefore, this work sets out to validate the hybrid LES/RANS method developed at NC State as applied to atmospheric re-entry flows. Furthermore, the method is extended to include thermal nonequilibrium effects, which are generally present in low density, high enthalpy conditions typical of re-entry environments.

The remainder of the thesis is organized as follows: first, the formulation of the governing equations for a mixture in full thermochemical nonequilibrium is presented in Chapter 2, followed by the corresponding numerical discretization in Chapter 3. Then, two different applications representative of hypersonic reentry flows are studied. In Chapter 4 data obtained from a series of experiments performed at the CUBRC LENS facility is used to assess the performance of the hybrid LES/RANS approach, and comparisons are also made with DES solutions obtained in [5] and with RANS results. In Chapter 5, the implementation of thermochemical nonequilibrium capabilities to our code is verified by modeling a 2D flow around a cylinder, and comparing results with the established Data Parallel Line Relaxation (DPLR) code from NASA [69]. Also, results are shown for a 3D case around a blunt body using RANS and LES/RANS in thermal and chemical nonequilibrium. Finally, a summary of the work and conclusions are presented in Chapter 6.
Chapter 2

Governing Equations

2.1 Flows in Thermal and Chemical Nonequilibrium

As a hypersonic vehicle enters the atmosphere, chemical and thermal nonequilibrium processes can take place if the time required for the process is on the same order of magnitude as the transit time across the region [26]. Such effects become important when the Damköhler $DAM$ number is of order 1. The Damköhler number is given by $DAM = t_{\text{res}}/t_{\text{chem}}$, where $t_{\text{res}}$ is the residence time of fluid particles in the region and $t_{\text{chem}}$ is the excitation and/or reaction time of a species. Moreover, when the $DAM$ is much greater than 1, the gas is said to be in a state of equilibrium, where the processes occur fast enough that the energy and mass fractions of a species are only functions of the local pressure and temperature. When $DAM$ approaches 0, the flow is said to be frozen [28].

From a microscopic point of view, the internal energy in a simple “dumbbell-like” gas molecule is due to contributions of translational, rotational and vibrational motions in space, and to the electronic energy provided by the kinetic energy of electrons around the nucleus and electromagnetic forces between the electrons and the nucleus. Therefore, the total energy for a gas molecule is given by the summation of all the contributions mentioned as:

$$e = e^{\text{trans}} + e^{\text{rot}} + e^{\text{vib}} + e^{\text{elec}} + e^{o}$$

(2.1)

where $e^{o}$ is the zero point energy of the molecule [4]. For an atomic species, the rotational and vibrational components would not be included in the total energy expression in Eq. 2.1. When a gas is said to be in thermal equilibrium, all the energy modes are governed by a single temperature $T$. However, thermal nonequilibrium describes the condition where all the energy modes cannot be described by the same temperature [26]. The different energy modes and chemical processes in a non-equilibrium flow are eventually driven towards equilibrium.
by the kinetics of the problem, however, equilibrium is achieved through collisions between particles. It takes on the order of 10 collisions to equilibrate translational and rotational energy modes. Therefore, these two modes are typically considered to be fully excited and governed by the same temperature for all practical purposes. However, the vibrational mode takes on the order of 10,000 collisions to reach equilibrium [28]. This large difference between the number of collisions to equilibrate of the translational/rotational and vibrational energy modes results in a state of thermal nonequilibrium. Furthermore, dissociation/recombination of molecules requires > 10,000 collisions to reach equilibrium.

Ahead of a blunt re-entry vehicle, the strong temperature and pressure jumps across the bow shock initiate the chemical reactions. More specifically, in an air atmosphere, dissociation of molecular oxygen occurs first, followed slowly by the dissociation of molecular nitrogen. This results in the creation of additional species such as nitrous oxide, atomic nitrogen, atomic oxygen, and in very high temperature cases, ionized species. When traveling in low enough densities and at high enough velocities (or total enthalpies), a state of vibrational non-equilibrium also results as the flow travels across the shock. Then as the flow expands rapidly around the shoulders of the vehicle, the flow’s vibrational energy pool remains essentially frozen. Accurate modeling of such phenomena is important for several reasons. First, chemical reactions occurring in the base region can affect the base pressure and even induce an additional pitching moment. This kind of pitching moment “anomaly” was observed in flights of the Space Shuttle, where chemical nonequilibrium effects contributed to an unexpected increase in pitching moment during flight [4]. Other important design considerations where nonequilibrium effects play an important role are: accounting for radiation in the base region for TPS design purposes, optical radiation in the wake, and wake electron densities, which affect radio communications [50].

Different models have been developed to account for thermal nonequilibrium. Lee [39] proposed a three temperature model where the translational and rotational modes are governed by a single temperature, and the vibrational and electronic modes are each governed by their own temperature. Accounting for a separate temperature for the electronic energy becomes important in flows where there is a significant degree of ionization. Another model, proposed by Park [48], assumes that the energy exchange between the electron translational mode and the vibrational mode is very fast, and therefore, they are governed by a single temperature, but still different from the translational/rotational temperature. This popular two temperature model is adopted in this work and is described in more detail throughout this chapter. Finally, a 5-species 5-reaction chemical kinetics model for air is adopted in this work, which is described in detail in section 2.4 of this chapter.
2.2 Navier-Stokes Equations

The general set of partial differential equations which describe the motion of an unsteady, viscous, compressible, continuum fluid are the Navier-Stokes equations. These governing equations are derived from conservation of mass, conservation of momentum and conservation of total energy. In this section, the Navier-Stokes equations are presented for a general three-dimensional flow composed of a mixture of $n_s$ species in thermochemical nonequilibrium. When considering a reactive mixture, the conservation of mass principle is applied to each individual species $n$, yielding a separate continuity equation for each species, which can be written in index notation as:

$$\frac{\partial \rho_n}{\partial t} + \frac{\partial [\rho_n (u_i + V_{n,i})]}{\partial x_i} = \dot{\omega}_n$$

(2.2)

where $\rho_n$ is the density of species $n$, and the mixture density can be obtained from $\rho = \sum_n \rho_n$. Also, $u_i, V_{n,i}, \dot{\omega}_n$ are the mixture velocity component $i$, the diffusion velocity of species $n$, and the chemical production term of species $n$, respectively. The conservation of momentum and conservation of total energy can be written as

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial t_{ij}}{\partial x_j}$$

$$\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_i} (\rho u_i H) + \frac{\partial}{\partial x_i} (\sum_{n=1}^{n_s} \rho_n V_{n,i} h_n) = \frac{\partial}{\partial x_i} (u_j t_{ij}) - \frac{\partial q_i}{\partial x_i}$$

(2.3)

where $E$ is the total energy per unit mass, $P$ is the mixture pressure, $H$ is the total enthalpy and $h_n$ is the specific enthalpy of species $n$. Furthermore, the specific enthalpy of the mixture is obtained from a weighted sum over all the species present as

$$h = \sum_{n=1}^{n_s} Y_n h_n$$

(2.4)

where the mass fraction of species $n$ is given by $Y_n = \rho_n / \rho$. The total enthalpy can be obtained from the total energy, pressure and density as follows

$$H = E + P/\rho$$

(2.5)

and the thermodynamic pressure of the mixture is obtained from the ideal gas law

$$P = \sum_{n=1}^{n_s} P_n = \sum_{n=1}^{n_s} \rho_n R_n T$$

(2.6)
where $T$ is the translational/rotational temperature of the mixture, and $R_n$ can be obtained from the universal gas constant $R_u$ and the species molecular weight $R_n = R_u/M_n$. According to the Stokes hypothesis, the viscous stress tensor $t_{ij}$ can be written as

$$t_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$  (2.7)

where $\mu$ is the molecular viscosity. The formulation of the heat flux vector assumes Fourier’s law, and is composed of contributions due to the translational temperature $T$, rotational temperature $T_r$, the vibrational temperature $T_v$, and the electron temperature $T_e$:

$$q_i = -k \frac{\partial T}{\partial x_i} - k_r \frac{\partial T_r}{\partial x_i} - k_v \frac{\partial T_v}{\partial x_i} - k_e \frac{\partial T_e}{\partial x_i}$$  (2.8)

where $k$, $k_r$, $k_v$, and $k_e$ are the respective thermal conductivities.

In general, the total energy per unit mass of a fluid is defined as the sum of the specific internal energy $e$ and the kinetic energy: $E = e + (1/2)u_iu_i$. When the mixture considered is in a state of thermal nonequilibrium, the internal energy can have contributions due to different energy modes, each of which (in general) is governed by a different temperature [37]:

$$e = \sum_{n=1}^{ns} Y_n e_n^{\text{trans}}(T) + \sum_{n=1}^{molec} Y_n e_n^{\text{rot}}(T_r) + \sum_{n=1}^{molec} Y_n e_n^{\text{vib}}(T_v) + \sum_{n=1}^{ns} Y_n e_n^{\text{elec}}(T_e) + \sum_{n=1}^{ns} Y_n h_n^o$$  (2.9)

where for each species $n$, $e_n^{\text{trans}}$ represents the translational energy, $e_n^{\text{elec}}$ is the electronic energy due to the kinetic and potential energy of electrons in orbit around the nucleus, $h_n^o$ is the formation enthalpy of species $n$, and $T$, $T_e$ are the representative translational and electronic temperatures, respectively. In addition, for diatomic molecules present in the mixture, a “dumbbell” representation of the molecule is adopted, and additional energy modes must be accounted for. In Eq. 2.9, $e_n^{\text{rot}}$ is the energy contribution due to rotational kinetic energy, $e_n^{\text{vib}}$ is the energy contribution due to the “spring-like” vibrations of the atoms in the molecule, and $T_r$ and $T_v$ are the corresponding representative temperatures of these energy modes [4].

It is common to assume that the rotational mode is fully excited, that it, the rotational energy mode equilibrates very rapidly with the translational mode, and therefore one can assume that they are governed by a single temperature ($T=T_r$). Similarly, it is often assumed that the electronic and vibrational energy modes are governed by a common temperature ($T_v=T_e$) [37]. This results in a two-temperature model for a gas in thermal nonequilibrium, where $T$ and $T_v$ govern the energy of the system through Eq. 2.9. In temperature ranges of practical interest, the electronic energy contribution is often small [64]. Therefore, this work neglects the electronic energy term, but it is presented in the formulation above for completeness. The vibrational
energy of the system is governed by an additional conservation equation:

\[
\frac{\partial}{\partial t} (\rho e^{\text{vib}}) + \frac{\partial}{\partial x_i} \left( \rho u_i e^{\text{vib}} \right) + \frac{\partial}{\partial x_i} \left( \sum_{n=1}^{n_s} \rho_n V_n e^{\text{vib}}_n \right) = -\frac{\partial q^{\text{vib}}_i}{\partial x_i} + \dot{\omega}_v
\]  

(2.10)

where \(\dot{\omega}_v\) is the vibrational energy source term, and the heat flux vector contribution is

\[
q^{\text{vib}}_i = -k \frac{\partial T_v}{\partial x_i}
\]  

(2.11)

The special case of a thermally perfect reacting gas can be recovered from the equations above by simply replacing all instances of \(T_v\) with \(T\). Furthermore, the special case for a non-reacting calorically perfect gas is recovered by neglecting all source terms and all terms involving \(T_v\) and \(e_v\). This results in only a single energy equation given in Eq. 2.3 and the internal energy given by Eq. 2.9 reduces to:

\[
e(T) = \sum_{n=1}^{n_s} Y_n e^{\text{trans}}_n (T) + \sum_{n=1}^{\text{molec}} Y_n e^{\text{rot}}_n (T) + \sum_{n=1}^{n_s} Y_n h_0^n
\]  

(2.12)

Under the assumptions presented for the two temperature model, the sum of the translational and rotational energy contributions can be modeled with a single heat capacity,

\[
e^{\text{trans}}_n (T) + e^{\text{rot}}_n (T) = C^{\text{tr}}_{v,n} T
\]  

(2.13)

where \(C^{\text{tr}}_{v,n}\) is the translational/rotational specific heat at constant volume of species \(n\). Note that in Eq. 2.13 the subscript \(v\) simply indicates the property at constant volume, and has no relation to the vibrational energy mode. The expressions for \(C^{\text{tr}}_{v,n}\) can be obtained from statistical thermodynamics by assuming a Boltzmann distribution of the atoms (or molecules) over all the energy levels of the system. This assumption is good for high temperatures (>5 K) such as those encountered in re-entry environments, however, at temperatures below 5 K, Bose-Einstein or Fermi-Dirac statistics must be considered [4]. The analysis adopting the Boltzmann distribution assumption yields \(C^{\text{tr}}_{v,n} = (3/2)R_n\) for atoms, and \(C^{\text{tr}}_{v,n} = (5/2)R_n\) for molecules. By employing principles from quantum mechanics and assuming the harmonic oscillator model for diatomic molecules, the vibrational energy of molecules can be calculated from:

\[
e^{\text{vib}}_n = \frac{R_n \theta_{v,n}}{\exp(\theta_{v,n}/T_v) - 1}
\]  

(2.14)

where \(\theta_{v,n}\) is the characteristic temperature of vibration of species \(n\), and selected values are listed in Appendix A. Even though all molecules are anharmonic oscillators in reality, the harmonic oscillator assumption yields good results and, in general, is used in most practical
applications when dealing with nonequilibrium flows [4].

2.3 Transport Properties

In this work, the Blottner curve fits [8] are used to compute the viscosity as a function of temperature \((T)\) for each species in the mixture,

\[
\mu_n(T) = 0.1 \exp[(A_n \ln T + B_n) \ln T + C_n] \tag{2.15}
\]

where the resulting viscosity values are in units of kg/m-sec, and selected values for each constant are listed in Appendix A. These curve fits are valid for temperatures below 10,000 K [37]. Using the computed molecular viscosities, the thermal conductivities for the different energy modes can be obtained for each species by using an Eucken relation,

\[
\begin{align*}
    k^{\text{trans}}_n &= \frac{5}{2} \mu_n C^{\text{trans}}_{v,n} \\
    k^{\text{rot}}_n &= \mu_n C^{\text{rot}}_{v,n} \\
    k^{\text{vib}}_n &= \mu_n C^{\text{vib}}_{v,n}
\end{align*}
\tag{2.16}
\]

where the corresponding constant-volume specific heats are given by

\[
\begin{align*}
    C^{\text{trans}}_{v,n} &= \frac{3}{2} R_n \\
    C^{\text{rot}}_{v,n} &= R_n \\
    C^{\text{vib}}_{v,n} &= R_n \left( \frac{\theta_{v,n}}{T_v} \right)^2 \left[ \exp(\theta_{v,n}/T_v) - 1 \right]^2
\end{align*}
\tag{2.17}
\]

In order to obtain the mixture’s viscosity and thermal conductivity, Wilke’s mixing rule is employed as follows,

\[
\begin{align*}
    \mu &= \sum_{n=1}^{n_s} \frac{\mu_n \chi_n}{\phi_n} \\
    k &= \sum_{n=1}^{n_s} \frac{k_n \chi_n}{\phi_n}
\end{align*}
\tag{2.18}
\]
\[ \phi_n = \sum_{n=1}^{n_s} \chi_n \left[ 1 + \sqrt{\frac{\mu_n}{\mu_r}} \sqrt{\frac{M_r}{M_n}} \right]^2 \sqrt{8 \left( 1 + \frac{M_n}{M_r} \right)} \]

(2.19)

\[ \chi_r = Y_r \left( \sum_{n=1}^{n_s} \frac{Y_n}{M_n} \right)^{-1} M_r \]

For certain cases considered in this work for a non-reacting calorically perfect gas, a constant Prandtl number assumption is used to compute thermal conductivity (instead of Eq. 2.16). When doing so, a constant Prandtl number of 0.72 is assumed, and thermal conductivity is computed as \( k = \sum_{n=1}^{n_s} \frac{Y_n C_{p,n}}{Pr} \), where \( C_{p,n} \) can be obtained from \( C_{p,n} = C_{v,n} + R_n \) or from polynomial curve fits such as those presented by McBride et al. [45].

The mechanism of species diffusion depends, in general, on temperature, pressure and species concentrations. However, pressure diffusion is usually very small, and thermal diffusion is also small when compared with diffusion driven by concentration gradients [4]. Therefore, we only consider diffusion due to concentration gradients in this work, and we obtain diffusive velocities by assuming a single diffusion coefficient for all species and adopting Fick’s law,

\[ V_{n,i} = -\frac{\mu}{Sc} \frac{\partial Y_n}{\partial x_i} \]

(2.20)

where \( Sc \) is the Schmidt number, which is assumed to be constant. In this study, we adopt a constant \( Sc \) of 0.5.

### 2.4 Chemical Kinetics

When considering a mixture in chemical nonequilibrium, the chemical source terms \( \dot{\omega}_n \) in Eq. 2.2 are obtained from chemical kinetics by considering a finite set of important chemical reactions. A single-step reaction can be written in the canonical form

\[ \sum_{i=1}^{ncmp} \nu'_i S_i \leftrightarrow \sum_{i=1}^{ncmp} \nu''_i S_i \]

(2.21)

where \( ncmp \) is the total number of compounds in the reaction, \( S_i \) is a molecule of the \( i \)-th species, \( \nu'_i \) is the stoichiometric coefficient corresponding to species \( i \) in the reactants, and \( \nu''_i \) is the stoichiometric coefficient corresponding to species \( i \) in the products [4]. The species source terms can be obtained for \( nr \) reactions from the law of mass action as

\[ \dot{\omega}_n = M_n \sum_{r=1}^{nr} (\nu''_{n,r} - \nu'_{n,r}) RR_r \]

(2.22)
where $M_n$ is the $n$-th species molecular weight, $RR_r$ is the net reaction rate of reaction $r$, and $\nu'_{n,r}$ and $\nu''_{n,r}$ are the stoichiometric coefficients corresponding to species $n$ in reaction $r$ in the products and reactants, respectively. For bimolecular exchange reactions of the form $A + B \rightleftharpoons C + D$, the reaction rate is of the form

$$RR_r = \frac{k_f,r}{k_b,r} \prod_{n=1}^{n_s} [S_n]^{\nu'_{n,r}} - \frac{k_b,r}{k_f,r} \prod_{n=1}^{n_s} [S_n]^{\nu''_{n,r}}$$  \hspace{1cm} (2.23)$$

where $[S_n]$ is the concentration (in moles/volume) of species $S_n$, and $k_{f,r}$ and $k_{b,r}$ are the forward and backward reaction rate constants, respectively. Similarly, when considering a dissociation reaction of the form $A + B + M \rightleftharpoons C + D + M$, where $M$ is a third body which facilitates the reaction, the net reaction rate is written as

$$RR_r = \left\{ \frac{k_f,r}{k_b,r} \prod_{n=1}^{n_s} [S_n]^{\nu'_{n,r}} - \frac{k_b,r}{k_f,r} \prod_{n=1}^{n_s} [S_n]^{\nu''_{n,r}} \right\} \sum_{n=1}^{n_s} [S_n](TB_{n,r})$$  \hspace{1cm} (2.24)$$

where the additional multiplier takes into account the collisions with all possible third bodies by including a third body efficiency factor $TB_{n,r}$ for each species in a reaction $r$. These third body efficiency factors are given in Appendix A for the chemistry model employed in this work. The reaction rate constants for each reaction are independent of concentrations and they depend only on temperature. Furthermore, the forward rate constant of each reaction can be written in Arrhenius form as

$$k_{f,r}(T_a) = C_{f,r}(T_a)^{\eta_r} \exp\left[-E_{a,r}/R_uT_a\right]$$  \hspace{1cm} (2.25)$$

where $T_a$ is an effective temperature used to evaluate the rate constant, $C_{f,r}$ is a constant specific to reaction $r$, $\eta_r$ is the pre-exponential factor, and $E_{a,r}$ is an activation energy [37]. The values for $C_{f,r},\eta_r$, and $E_{a,r}$ specific to each reaction are typically measured experimentally [38], and the values used for this work are presented in Appendix A. In Park’s model, he proposes that forward rate coefficients for dissociation reaction are a function of both translational/rotational temperature ($T$) and vibrational temperature ($T_v$). This idea, termed preferential dissociation, proposes that molecules are more easily dissociated when they are already vibrationally excited. Therefore, Park [50] defines an average temperature defined as:

$$T_a = \sqrt{TT_v}$$  \hspace{1cm} (2.26)$$

which is used to evaluate only the forward rate constants $k_{f,r}(T_a)$ for dissociation reactions. For the remaining reactions $T_a = T$.

To obtain the backward reaction rate constant of each reaction, one can take advantage of the following relation between the forward rate constant, backward rate constant and equilibrium
constant $K_{eq}$:

$$K_{eq} = \frac{k_{f,r}(T_a)}{k_{b,r}(T)}$$

(2.27)

where the equilibrium constant can be obtained from curve fits or from chemical thermodynamics by minimizing the change in Gibbs free energy [38]. However, the equilibrium constant should be evaluated at the translational/rotational temperature $T$ [50].

### 2.4.1 Park 1985 Reaction Mechanism

In this work, we implement a 5-species chemical model for high temperature air by Park [49] where only the five most important chemical reactions are considered. The only five species considered are $N_2$, $O_2$, NO, N and O. The reaction mechanism is valid for temperatures below 9000 K [4] and it is shown below:

$$
\begin{align*}
N_2 + M & \leftrightarrow N + N + M \\
O_2 + M & \leftrightarrow O + O + M \\
NO + M & \leftrightarrow N + O + M \\
N_2 + O & \leftrightarrow NO + N \\
NO + O & \leftrightarrow O_2 + N
\end{align*}
$$

(2.28)

The first three reactions are dissociation reactions, while the remaining two are bimolecular exchange reactions which are commonly referred to as the Zeldovich reactions. The third body ($M$) involved in the three dissociation reactions can be any of the species in the mixture, and its role is to absorb the energy necessary for the reaction to take place. This basic reaction mechanism neglects the ionization of species which is certainly possible at high temperatures. However, future work shall include more complex reaction mechanisms for high temperature air such as Park’s 11-species model or Dunn and Kang’s model [4].

In order to obtain the equilibrium constant $K_{eq}$, we use the curve fit proposed by Park [49] of the form:

$$K_{eq}(T) = \alpha_r exp(A_{1r} + A_{2r}z + A_{3r}z^2 + A_{4r}z^3 + A_{5r}z^4)$$

(2.29)

where $z = 1000/T$ and $\alpha_r = 1000$ for dissociation reactions and 1.0 for exchange reactions. The values of the coefficients for each of the 5 reactions considered are presented in Appendix A.

### 2.4.2 Vibrational Energy Source Term

For a reactive flow in vibrational nonequilibrium, two different contributions must be considered to form the vibrational energy source term in Eq. 2.10. The first contribution is simply due to the creation of new molecular species, which add to the vibrational energy pool. This term can
be obtained directly from the chemical source terms of molecular species,

\[
\dot{\omega}_{\text{v,spec}} = \sum_{n=1}^{\text{molec}} \dot{\omega}_n e_n^{\text{vib}} \tag{2.30}
\]

In addition, vibrational energy is also created/destroyed due to the transfer of energy between the different energy modes of a particle. For example, when two molecules collide, there could be energy exchanges between the translational and vibrational modes, between the rotational and vibrational modes, and even between two different vibrational modes [37]. However, under the two temperature model assumptions, we only consider energy coupling between the translational/rotational and vibrational modes. This term can be modeled by using the Landau-Teller equation:

\[
\dot{\omega}_{\text{tr-v}} = \sum_{n=1}^{\text{molec}} \rho_n \frac{e_n^{\text{vib}} - e_n^{\text{vib,Eq}}}{\tau_n^{\text{vib}}} \tag{2.31}
\]

where \(e_n^{\text{vib,Eq}}\) is obtained by evaluating the vibrational energy \(\text{Eq. 2.14}\) at the translational/rotational temperature \(T\). This model is derived by making three major assumptions about the vibrational energy levels of molecules. It is assumed that the vibrational energy levels are populated according to a Boltzmann distribution, that only transitions occurring between two neighboring vibrational energy states are considered, and that the rate of these transitions is proportional to the vibrational quantum number [50]. The vibrational relaxation time for each species can be obtained from Millikan and White:

\[
\tau_n^{\text{vib}} = \sum_{r=1}^{n_s} \frac{\chi_r}{\left( \sum_{r=1}^{n_s} \chi_r^{\text{vib}} \right)} \tag{2.32}
\]

where \(\chi_r\) was defined in \(\text{Eq. 2.19}\) and

\[
\tau_{n,r}^{\text{vib}} = \frac{1}{p} \exp \left[ A_{n,r} \left( T^{-1/3} - 0.015 \mu_n^{1/4} \right) \right] - 18.42
\]

\[
A_{n,r} = 1.16 \times 10^{-3} \mu_n^{1/2} \theta_n^{4/3}
\]

where \(p\) is the pressure in units of atmospheres. The equivalent molecular weight \(\mu_{n,r}\) is given by:

\[
\mu_{n,r} = \frac{M_n M_r}{M_n + M_r} \tag{2.34}
\]

The relaxation times obtained from \(\text{Eq. 2.32}\) are a good approximation for temperatures up to 5000 K. For higher temperatures, additional corrections must be added to the relaxation time since the three aforementioned assumptions which were used to derive the Landau-Teller equation become invalid [50]. Finally, adding the two different sources of vibrational energy...
considered, the net vibrational energy production term is obtained

\[ \dot{\omega}_v = \dot{\omega}_{v,\text{spec}} + \dot{\omega}_{tr-v} \]  

(2.35)

2.5 Reynolds-Averaged Navier-Stokes Equations

Advances in the field of turbulence data back to the late 1800’s, however, the first turbulence model was not developed until 1930 by von Karman [65]. The first attempts at modeling the turbulence problem focused on solving the Reynolds-Averaged Navier-Stokes (RANS) equations. Currently, RANS models are still the simplest and least expensive way to model turbulence, and they are the most popular choice for practical applications.

Reynolds averaging can be accomplished by either time averaging, spatial averaging, or ensemble averaging. In this section, the RANS equations are developed using time averaging. To take into account the flow fluctuations due to turbulence, the instantaneous velocity \( u_i(x, t) \) can be decomposed into a mean velocity \( U_i(x, t) \) and a fluctuating component \( u'_i(x, t) \) as [65]:

\[ u_i(x, t) = U_i(x, t) + u'_i(x, t) \]  

(2.36)

where \( x \) represents a spatial dimension and \( t \) is the time variable. Also, the Reynolds (time) average of a generic variable \( X \) is defined as

\[ \bar{X}(x, t) = \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} X(x, t) dt \]  

(2.37)

and it can be shown that \( \bar{u}'_i(x, t) = 0 \). When dealing with compressible flows, density and temperature fluctuations must also be accounted for, which can usually be neglected for incompressible flows. Therefore introducing a density-weighted average, named Favre average, the formulation of the equations can be simplified. The Favre averaging of a generic variable \( X \) is defined as:

\[ \tilde{X}(x, t) = \frac{1}{\bar{\rho}} \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} \rho(x, t) X(x, t) dt \]  

(2.38)

where \( \rho \) is density and \( \bar{\rho} \) is the Reynolds-averaged density. In a fashion similar to that proposed by Eq. 2.36, we can decompose the instantaneous velocity as a sum of a Favre averaged component \( \tilde{u}_i(x, t) \) and a fluctuating part \( u''_i(x, t) \):

\[ u_i(x, t) = \tilde{u}_i(x, t) + u''_i(x, t) \]  

(2.39)

To obtain the mass averaged mean conservation equations, a combination of Reynolds and
Favre averaging is used as follows,

\[ u_i = \bar{u}_i + u_i'' \]
\[ V_{n,i} = \bar{V}_{n,i} + V_{n,i}'' \]
\[ Y_n = \bar{Y}_n + Y_n'' \]
\[ \dot{\omega}_n = \bar{\dot{\omega}}_n + \dot{\omega}_n' \]
\[ \rho = \bar{\rho} + \rho' \]
\[ p = \bar{p} + p' \]
\[ h = \bar{h} + h'' \]
\[ e = \bar{e} + e'' \]
\[ T = \bar{T} + T'' \]
\[ \dot{q}_i = q_{L,i} + q_i' \]

where \( q_i \) is the heat flux vector, \( q_{L,i} \) is the laminar component of the heat flux vector, and for the two-temperature model, it is composed of translational/rotational and vibrational components as:

\[ q_{L,i} = q_{tr,L,i} + q_{vib,L,i} \]  \hspace{1cm} (2.41)

and the ideal gas law in terms of mean density is now \( P = \bar{\rho}RT \).

Substituting the expressions given by Eq. 2.40 into the instantaneous Navier-Stokes equations and mass-averaging, the Favre-averaged Navier-Stokes equations for a multi-component mixture in thermochemical nonequilibrium are obtained:

\[ \frac{\partial \bar{\rho}_n}{\partial t} + \frac{\partial}{\partial x_i} \left[ \bar{\rho}_n (\bar{u}_i + \bar{V}_{n,i}) \right] = \bar{\dot{\omega}}_n \] \hspace{1cm} (2.42)

\[ \frac{\partial (\bar{\rho}\bar{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho}\bar{u}_i\bar{u}_j) = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} (\bar{t}_{ij} + \bar{\rho}\tau_{ij}) \] \hspace{1cm} (2.43)

\[ \frac{\partial}{\partial t} (\bar{\rho}E) + \frac{\partial}{\partial x_j} (\bar{\rho}\bar{u}_jH) = \frac{\partial}{\partial x_j} \left( -q_{L,j} - q_{T,j} + \bar{t}_{ij}\bar{u}_i\bar{u}_j' - \frac{\bar{\rho}u_j'u_i'u_i''}{2} \right) + \frac{\partial}{\partial x_j} [\bar{u}_i (\bar{t}_{ij} - \bar{\rho}\tau_{ij})] \] \hspace{1cm} (2.44)

where \( \bar{\rho}\tau_{ij} = -\bar{\rho}u_j'u_i'' \) is the Favre averaged Reynolds stress tensor. Furthermore, the well-known Boussinesq eddy viscosity approximation is also assumed, so we go one step further to define

\[ \bar{\rho}\tau_{ij} = 2\mu_T \left( S_{ij} - \frac{1}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \bar{\rho}k\delta_{ij} \] \hspace{1cm} (2.45)
where \( \mu_T \) is the turbulent eddy viscosity. We also define the turbulent kinetic energy per unit volume of the turbulent fluctuations \( k \) as:

\[
\bar{\rho}k \equiv \rho u''_i u''_i / 2 \tag{2.46}
\]

Additional definitions are also worth noting for completeness:

\[
E = \ddot{\epsilon} + \frac{1}{2} \ddot{u}_i \ddot{u}_i \\
H = \ddot{h} + \frac{1}{2} \ddot{u}_i \ddot{u}_i \tag{2.47}
\]

In this work, the turbulent heat flux vector includes a contribution due to the vibrational temperature gradients, and the thermal conductivities are evaluated using a constant turbulent Prandtl number assumption:

\[
q_{T,j} = q_{T,j}^{tr} + q_{T,j}^{vib} = \mu_{Pr} \left( C_{p}^{tr} \frac{\partial T}{\partial x_j} + C_{p}^{vib} \frac{\partial T_v}{\partial x_j} \right) \tag{2.48}
\]

where the values of \( \text{Pr} \) and \( \text{Pr}_T \) are assumed to be 0.72 and 0.9. Laminar and turbulent Schmidt numbers are also assumed to be constant and a value of 0.5 is used for both. Finally, we also neglect the molecular diffusion and turbulent transport of turbulence kinetic energy terms in this work, which are \( \bar{t}_{ij} u''_i \) and \( \rho u''_i u''_j / 2 \) in Eq. 2.44, respectively.

### 2.5.1 Menter’s \( k - \omega \) BSL model

Applying all the turbulence closure approximations defined in the previous section, there are still two unknowns remaining: \( k \) and \( \mu_T \). In this work, we use Menter’s two-equation \( k - \omega \) Baseline (BSL) model to close the problem. This model introduces two additional equations which allow solving for the two remaining unknowns. The BSL model is a combination of the Wilcox \( k - \omega \) model and the \( k - \epsilon \) model. The transition from one model to the other is achieved by a blending function which turns on the Wilcox \( k - \omega \) model near walls, where the \( k - \epsilon \) model presents a lack of sensitivity to adverse pressure gradients, and switches to the \( k - \epsilon \) in the wake region of the boundary layer, where the Wilcox \( k - \omega \) typically suffers from sensitivity to the freestream specification of the specific dissipation rate (\( \omega \)) [46]. The Menter BSL model consists of one equation for the turbulence kinetic energy \( k \), and an additional equation for the
specific dissipation rate $\omega$:

$$\frac{D\rho k}{Dt} = \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_k \mu_T) \frac{\partial k}{\partial x_j} \right]$$

$$\frac{D\rho \omega}{Dt} = \frac{\gamma}{\nu_T} \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_T) \frac{\partial \omega}{\partial x_j} \right] + 2 \rho (1 - F_1) \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$$

(2.49)

where the last term in the $\omega$ equation is termed the cross diffusion term, and it is a result of transforming the original $\epsilon$ equation into an equation in terms of $\omega$. The model uses the following definition for eddy viscosity:

$$\nu_T = \frac{\mu_T}{\rho} = \frac{k}{\omega}$$

(2.50)

and the blending function is given by

$$F_1 = \tanh(\text{arg}_1)$$

$$\text{arg}_1 = \min \left( \max \left( \frac{\sqrt{k}}{0.09 \omega y}, \frac{500 \nu}{y^2 \omega} \right), \frac{4 \rho \sigma_\omega k}{CD_k \omega y^2} \right)$$

(2.51)

and

$$CD_k \omega = \max \left( 2 \rho \sigma_\omega \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 10^{-20} \right)$$

The model constants are each calculated by blending the constant’s value from the original Wilcox $k - \omega$ model with those from the standard $k - \epsilon$ model according to:

$$\phi = F_1 \phi_1 + (1 - F_1) \phi_2$$

(2.52)

where $\phi$ represents any one of the BSL constants, $\phi_1$ is the corresponding value from the $k - \omega$ model, and $\phi_2$ is the corresponding value from the $k - \epsilon$ model. The constants are listed in Table 2.1.

### 2.6 Filtered Navier-Stokes Equations

An alternative turbulence modeling approach, termed Large Eddy Simulation (LES), provides higher fidelity than RANS models. The development of LES techniques began in the 1960’s with the introduction of the Smagorinsky model. Smagorinsky was an American meteorologist who developed an LES approach in hopes of studying atmospheric and oceanic flows [41]. Ever since, significant advances have been made in LES methods and it is still very much an evolving
Table 2.1: Constants for Menter’s BSL model

<table>
<thead>
<tr>
<th>Constant</th>
<th>Wilcox $k - \omega , (\phi_1)$</th>
<th>Standard $k - \epsilon , (\phi_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_k$</td>
<td>0.5000</td>
<td>1.0000</td>
</tr>
<tr>
<td>$\sigma_\omega$</td>
<td>0.5000</td>
<td>0.8560</td>
</tr>
<tr>
<td>$\beta$</td>
<td>0.0750</td>
<td>0.0828</td>
</tr>
<tr>
<td>$\beta^*$</td>
<td>0.0900</td>
<td>0.0900</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>0.5532</td>
<td>0.4404</td>
</tr>
</tbody>
</table>

field. LES works by filtering the instantaneous Navier-Stokes equations presented in Eq. 2.2 and Eq. 2.3, resulting in the filtered Navier-Stokes Equations. This approach allows us to resolve the larger scales of turbulence while modeling the effects of the smaller turbulence scales (which cannot be directly resolved) using a subgrid scale (SGS) model. Similar to the development of the RANS equations, the instantaneous velocity $u_i$ can be decomposed into a resolved scale $\hat{u}_i$ and a subgrid scale $u_i^{SGS}$ as:

$$u_i = \hat{u}_i + u_i^{SGS}$$ (2.53)

In this work, the resolvable-scale velocity is obtained by using a volume-average box filter given by [65]

$$\hat{u}_i(x, t) = \frac{1}{\Delta^3} \int_{x-\Delta x/2}^{x+\Delta x/2} \int_{y-\Delta y/2}^{y+\Delta y/2} \int_{z-\Delta z/2}^{z+\Delta z/2} u_i(\xi, \eta, \zeta, t) d\xi d\eta d\zeta$$ (2.54)

where the filter width $\Delta$ used is defined as

$$\Delta = \sqrt[3]{\Delta x \Delta y \Delta z}$$ (2.55)

and the subgrid scale velocity can be obtained from $u_i^{SGS} = u_i - \hat{u}_i$.

After filtering the instantaneous Navier Stokes equations, the resulting equations are of the same form as those obtained for the RANS equations in Eq. 2.42-Eq. 2.44. However, a subgrid scale stress tensor $\tau^{SGS}_{ij}$ appears in the equations instead of the Favre-averaged Reynolds stress tensor in the RANS equations. Closing the problem then involves finding a way to model this SGS stress tensor. Wilcox [65] points out that “subgrid scales constitute a significant portion of the turbulence spectrum, which highlights the importance of selecting an appropriate SGS model. In general, the main challenges that the SGS model must address are: using properties of the resolved scales to model effects of the subgrid scales, and determining what the interactions are between the subgrid scales and the resolved scales and how to model them. In reality, there is energy being transferred from the resolved scales to the SGS and vice versa, however, most
approaches neglect energy transfers from the SGS to the resolved scales and only model the cascade going from the larger resolved scales to the SGS [53]. In the present work, the LES component of our hybrid turbulence model uses the algebraic model of Lenormand et al. [40] for the subgrid eddy viscosity,

\[ \nu_{T,SGS} = C_M S^{1/2} (q^2)^{1/4} \Delta^{3/2} \quad C_M = 0.06 \]  

(2.56)

where \( q^2 \) is a measure of the subgrid kinetic energy and \( S \) is the vorticity vector. Additional details about the hybrid LES/RANS model are presented in section 2.7.

2.7 Hybrid LES/RANS Model

The idea behind a hybrid LES/RANS approach is to resolve the largest turbulence scales using LES, while modeling the smaller near-wall scales using a RANS model. The LES/RANS model used in this approach is based on Menter’s BSL model presented in section 2.5.1. One of the unique features of our particular hybrid method is how the model detects where to shift from RANS to LES. This is achieved by using the Boussinesq eddy-viscosity formulation and redefining \( \mu_T \) as

\[ \mu_T = \rho \left[ \Gamma \frac{k}{\omega} + (1 - \Gamma) \nu_{T,SGS} \right] \quad (2.57) \]

where the transition is made possible by a blending function which is continuous in both space and time, and its orignial form is given by

\[ \Gamma = \frac{1}{2} \left( 1 - \tanh \left[ 15 \left( \frac{1}{\lambda^2} - 1 \right) \right] \right) \quad (2.58) \]

The value of \( \lambda \) is a ratio of outer to inner length scales:

\[ \lambda = \frac{l_{out}}{l_{inn}} = \sqrt{\frac{10 \omega + k + k_R}{\bar{C}_\mu^{1/2} \bar{\omega} \kappa d}} \quad (2.59) \]

where \( \nu \) is the kinematic viscosity, \( k_R \) is the resolved kinetic energy, \( \kappa \) is the von Kármán constant, \( d \) is the distance form the nearest wall, \( C_\mu \) is 0.09, and values with a bar over them indicate ensemble averaged values. In the end, because only outer and inner boundary layer information is used, this approach results in a blending function which is independent of grid scale and does not require a problem-specific calibration [24]. This method of blending is very different from Detached Eddy Simulation and other hybrid schemes, where the grid spacing is used to define (or prevent) transition from RANS to LES near walls. Furthermore, because the method is intended to transition inside the boundary layer, it allows for the LES model to
resolve turbulent structures in the outer wake-like region of the boundary layer.

### 2.7.1 Modified Blending Function

Designing a grid which minimizes the total computational workload, but still provides sufficient resolution in areas of interest, is one of the main challenges with high fidelity approaches. If the boundary layer spacing at any wall is not fine enough, problems may arise due to the grid-independent formulation of the blending function described in the previous section. Because this original blending function depends solely on boundary layer properties, the model could switch from RANS to LES in regions where the grid resolution is not enough to resolve turbulent structures using LES. To address this problem, a grid scale correction term is added to the length scale ratio $\lambda$, which pushes the LES/RANS transition point to the edge of the boundary layer when the grid size is significantly larger than the outer length scale. The change is made by redefining $\lambda$ as given by Eq. 2.59 and introducing a function $g(l_{out})$ as follows:

$$\lambda = \frac{l_{out}g(l_{out})}{l_{inn}}, \quad g(l_{out}) = \min \left[ 10, \max \left( 1, \frac{1}{2} \frac{\Delta_{max}}{l_{out}} \right) \right]$$

(2.60)

where $\Delta_{max}$ is the maximum grid spacing over the three coordinate directions. The improvements achieved by using this “modified” blending function formulation will be assessed in chapter 4.
Chapter 3

Numerical Formulation

Even though certain assumptions and simplifications of the Navier-Stokes equations can produce analytical solutions for very simple problems, there is currently no analytical solution to the complete set of equations. Therefore, for practical applications, the system of equations must be framed numerically in order to solve the system by computational approaches. There have been many different numerical formulations to the Navier-Stokes equations proposed, and in the end, one must decide which is the “best” formulation for the types of problems being considered. However, each decision made during the discretization and formulation of the equations will impact the method’s speed, computational cost, stability, accuracy, amount of dissipation, etc.

In the present work, the three-dimensional, unsteady, compressible Navier-Stokes equations for a gaseous mixture in thermochemical nonequilibrium are solved using North Carolina State University’s REACTMB solver. REACTMB is a finite volume solver for use on block-structured grids. Inviscid fluxes are discretized using Edwards’ Low Diffusion Flux Splitting Scheme [17], viscous fluxes are computed using 2nd order central differences, and a Crank-Nicholson time discretization with a planar relaxation subiteration procedure is employed for time advancement.

3.1 Finite Volume Discretization

By discretizing a physical domain into smaller control volumes, the finite volume method solves the integral form of the governing equations in each individual volume. This method is popular since it can be easily applied to domains with highly irregular shapes, coordinate transformations are not required (unlike the finite difference method) for curvilinear geometries, the “conserved” quantities (mass, momentum, energy) are automatically conserved across cell boundaries, and the implementation is very intuitive in nature [61]. The first step in the formulation involves writing the 3D Navier-Stokes equations in conservative form and integrating
them over an arbitrary control volume of volume $\Omega$ and surface area $\Gamma$. This results in the following system,

$$
\int_{\Omega} \frac{\partial U}{\partial t} d\Omega + \int_{\Omega} \frac{\partial F_i}{\partial x_i} d\Omega + \int_{\Omega} \frac{\partial G_i}{\partial x_i} d\Omega = \int_{\Omega} W_i d\Omega \quad (3.1)
$$

where $U$ is the vector of conserved variables, $F_i$ is the inviscid flux vector, $G_i$ is the vector of viscous fluxes, $W_i$ contains the source terms, and the terms have been written in index notation where for a 3D case, $i=1,2,3$ correspond to the three coordinate directions. Applying the Green-Gauss theorem to the two integrals in Eq. 3.1 involving $F_i$ and $G_i$, we can then rewrite the expression in the following form,

$$
\int_{\Omega} \frac{\partial U}{\partial t} d\Omega + \int_{\Gamma} F_i n_i d\Gamma + \int_{\Gamma} G_i n_i d\Gamma = \int_{\Omega} W_i d\Omega \quad (3.4)
$$

Finally the discrete form of Eq. 3.4 can be approximated at a particular cell $c$ as

$$
\frac{\Delta U_c}{\Delta t} + \sum_{k=faces} (F_i n_i)_{k,c} \Gamma_{k,c} + \sum_{k=faces} (G_i n_i)_{k,c} \Gamma_{k,c} = W_i \Omega_c \quad (3.5)
$$
3.2 Low-Diffusion Flux-Splitting Scheme

In order to evaluate the second term (inviscid fluxes) in Eq. 3.5, the value of each component of the vector \( \mathbf{F}_i \) must be evaluated at each of the faces of the control volume being considered. One popular way to evaluate interface fluxes is employing a flux splitting approach. The idea behind flux vector splitting is to split the flux terms in a way which takes into account the way (and direction) information propagates. The splitting is carried out by means of the structure of the eigenvalues of the system, or by assuming certain behaviors [61]. In this work, viscous fluxes are computed using a second order central difference, and inviscid fluxes are evaluated using Edward’s Low-Diffusion Flux-Splitting Scheme (LDFSS). This method is considered a hybrid upwind scheme formulated as a flux splitting scheme, which is robust in capturing strong shocks, but combines some of the accuracy of flux-difference approaches when capturing shear layers [17]. Using this approach, the inviscid flux vector in Eq. 3.5 is split as follows:

\[
\mathbf{F} = \mathbf{F}^c + \mathbf{F}^p = \Gamma (\rho \mathbf{U} \mathbf{E}^c + p \mathbf{E}^p)
\]

\[
\mathbf{E}^c = \begin{bmatrix}
Y_1 \\
\vdots \\
Y_{n_{sp}} \\
u_1 \\
u_2 \\
u_3 \\
H \\
e^{vib}
\end{bmatrix} \quad \mathbf{E}^p = \begin{bmatrix}
0 \\
\vdots \\
0 \\
n_x \\
n_y \\
n_z \\
0 \\
0
\end{bmatrix}
\]

where \( \mathbf{F}^c \) is the convective contribution and \( \mathbf{F}^p \) the pressure component. In addition, \( \Gamma \) is the face area and \( \mathbf{U} \) is given by \( \mathbf{U} = u_1 \mathbf{n}_1 + u_2 \mathbf{n}_2 + u_3 \mathbf{n}_3 \) where \( \mathbf{n}_i \) is the unit vector normal to the cell face. The interface value \( \mathbf{E}^c_{1/2} \) is then obtained by using information from the left (L) and right (R) states as follows,

\[
\mathbf{E}^c_{1/2} = a_{1/2} \left[ \rho_L C^+ \mathbf{E}^c_L + \rho_R C^- \mathbf{E}^c_R \right]
\]

where

\[
a_{1/2} = \frac{1}{2} (a_L + a_R)
\]

\[
C^+ = C^+_{VL} - M^+_{1/2} \quad , \quad C^- = C^-_{VL} + M^-_{1/2}
\]

\[
C^+_{VL} = a_L^+(1.0 + \beta_L)M_L - \beta_L M^+_L
\]

\[
C^-_{VL} = a_R^-(1.0 + \beta_R)M_R - \beta_R M^-_R
\]
\[ M_{1/2}^+ = M_{1/2} \left( \frac{2p_R}{p_R + p_L} - \delta \frac{|p_L - p_R|}{p_L} \right) \]  
\[ (3.13) \]

\[ M_{1/2}^- = M_{1/2} \left( \frac{2p_L}{p_R + p_L} - \delta \frac{|p_L - p_R|}{p_R} \right) \]  
\[ (3.14) \]

\[ \alpha_{L/R}^\pm = \frac{1}{2} \left[ 1.0 \pm \text{sign} \left( M_{L/R} \right) \right] \]  
\[ (3.15) \]

\[ \beta_{L/R} = -\max \left[ 0.0, 1.0 - \int \left( |M_{L/R}| \right) \right] \]  
\[ (3.16) \]

\[ M_{L/R}^\pm = \pm \frac{1}{4} \left( M_{L/R} \pm 1.0 \right)^2 \]  
\[ (3.17) \]

\[ M_{1/2} = \frac{1}{4} \beta_{L/R} \left( \sqrt{\frac{1}{2} \left( M_L^2 + M_R^2 \right)} - 1.0 \right) \]  
\[ (3.18) \]

\[ M_{L/R} = \frac{1}{a_{1/2}} \left[ \hat{n}_1 u_{1,L/R} + \hat{n}_2 u_{2,L/R} + \hat{n}_3 u_{3,L/R} \right] \]  
\[ (3.19) \]

where a value of 2 was used for \( \delta \) in Eq. 3.13 and Eq. 3.14. Finally, the pressure contribution is given by

\[ E_{1/2}^p = E^p \left[ D_{L,R}^p p_L + D_{L,R}^p p_R \right] \]  
\[ (3.20) \]

\[ D_{L/R}^\pm = \alpha_{L/R}^\pm \left[ 1.0 + \beta_{L/R} \right] - \beta_{L/R} \bar{P}_{L/R}^\pm \]  
\[ (3.21) \]

\[ \bar{P}_{L/R}^\pm = \frac{1}{4} \left( M_{L/R} \pm 1.0 \right)^2 \left( 2.0 \mp M_{L/R} \right) \]  
\[ (3.22) \]

### 3.3 Extension of Fluxes to Higher Order

Inviscid fluxes are extended to higher order by using the piecewise parabolic method (PPM) of Colella and Woodward [11] or a total variation diminishing (TVD) scheme. Using the present formulation, the left and right states at a cell interface are calculated as:

\[ V_{L,i+1/2} = \left( 1 - f_i^P \right) V_{L,i+1/2}^H + f_i^P V_i \]  
\[ (3.23) \]

\[ V_{R,i+1/2} = \left( 1 - f_i^P \right) V_{R,i+1/2}^H + f_i^P V_{i+1} \]  
\[ (3.24) \]

where \( V = [p, u, v, w, T, k, \omega, T_v]^T \) represents the vector of primitive variables, \( V_{R,i+1/2}^H \) and \( V_{L,i+1/2}^H \) are high order interpolants at the right and left states of the cell interface \( i + 1/2 \), and \( f_i^P \) is a pressure limiter defined as:

\[ f_i^P = 1.25 \left[ \max \left( \frac{|\Delta^2 p|}{|\Delta^2 p| + \bar{p}}, 0.2 \right) - 0.2 \right] \]  
\[ (3.25) \]
This limiter reduces the scheme’s order to first when the pressure field curvature term $|\Delta^2 p|$ is large. The higher-order interpolants are constructed by using an average cell value $V_{i+1/2}^c$, a monotone interpolant value $V_{i+1/2}^M$ obtained from the PPM or TVD scheme, and a blending function $f_{i+1/2}^D$:

$$V_{L,i+1/2}^H = V_{i+1/2}^c + f_{i+1/2}^D \left( V_{i+1/2}^M - V_{i+1/2}^c \right)$$

(3.27)

$$V_{R,i+1/2}^H = V_{i+1/2}^c + f_{i+1/2}^D \left( V_{i+1/2}^M - V_{i+1/2}^c \right)$$

(3.28)

The blending function is computed by using the pressure limiter given by Eq. 3.25 and the vorticity/divergence function of Ducros et al. [12] such as:

$$f_{i+1/2}^D = \max \left( f_i^P, f_{i+1}^P, f_i^{Ducros}, f_{i+1}^{Ducros} \right)$$

(3.29)

$$f_i^{Ducros} = \frac{\left( \nabla \cdot \vec{V} \right)^2}{\left( \nabla \cdot \vec{V} \right)^2_i + |\nabla \times \vec{V}|^2 + \epsilon^2_i}, \quad \epsilon = 1 \times 10^{-8} V_\infty / \max(\Delta x \Delta y \Delta z)$$

(3.30)

By becoming active in regions of high vorticity, the Ducros blending function limits the dissipation introduced by the monotonic reconstruction scheme in regions where turbulence scales can be resolved. The averaging operator implemented yields a fourth-order central difference method on uniform meshes, and is defined as:

$$V_{i+1/2}^c = \frac{7}{12} (V_i + V_{i+1}) - \frac{1}{12} (V_{i+2} - V_{i-1})$$

(3.31)

### 3.4 Time Advancement

The full compressible Navier-Stokes equations are a set of mixed character (hyperbolic-parabolic) partial differential equations which can be advanced in time by either explicit or implicit schemes. Explicit schemes are, in general, easier to implement but the time step is very limited by CFL requirements for stability, even more so for reactive flows where the time scales associated with the chemistry processes are extremely small. On the other hand, implicit schemes involve more computational effort in terms of storage and solving large matrix systems, but they are stable for very large CFL numbers and allow the solution to evolve much quicker. In this work, an implicit Crank-Nicholson formulation of the unsteady Navier-Stokes equations is used to advance the solution in time. In order to simplify the implicit formulation, the Navier-Stokes
The equations given by Eq. 3.1 to Eq. 3.3, are rearranged as follows:

\[
\frac{\partial U}{\partial t} \Omega + \sum_{k=i\text{faces}} (\bar{E} \cdot n\Gamma)_k + \sum_{k=j\text{faces}} (\bar{F} \cdot n\Gamma)_k + \sum_{k=k\text{faces}} (\bar{G} \cdot n\Gamma)_k = W\Omega \tag{3.32}
\]

where

\[
\bar{E} = F_1 + G_1 , \quad \bar{F} = F_2 + G_2 , \quad \bar{G} = F_3 + G_3 \tag{3.33}
\]
as previously defined in Eq. 3.1 and Eq. 3.3, where the indices 1,2,3 correspond to the x,y and z direction vectors, respectively. The Crank-Nicholson formulation is as follows:

\[
\Omega \frac{U^{n+1} - U^n}{\Delta t} + \frac{1}{2} [R(V^{n+1}) + R(V^n)] = 0 \tag{3.34}
\]

where \( U \) is the vector of conserved variables, \( V \) is the primitive variables vector, \( n \) indicates the time level, and \( R \) is the steady residual given at a time \( n \) by

\[
R(V^n) = \sum_{k=i\text{faces}} (\bar{E}(V^n) \cdot n\Gamma)_k + \sum_{k=j\text{faces}} (\bar{F}(V^n) \cdot n\Gamma)_k + \sum_{k=k\text{faces}} (\bar{G}(V^n) \cdot n\Gamma)_k - \Omega W^n \tag{3.35}
\]

Evaluating the fluxes at their respective cell interfaces, further simplification of Eq. 3.34 yields,

\[
\Omega \frac{U^{n+1} - U^n}{\Delta t} + \frac{1}{2} \left[ (\bar{E}^{n+1}_{i+1/2,j,k} - \bar{E}^{n+1}_{i-1/2,j,k}) + (\bar{E}^n_{i+1/2,j,k} - \bar{E}^n_{i-1/2,j,k}) \right] + \frac{1}{2} \left[ (\bar{F}^{n+1}_{i,j+1/2,k} - \bar{F}^{n+1}_{i,j-1/2,k}) + (\bar{F}^n_{i,j+1/2,k} - \bar{F}^n_{i,j-1/2,k}) \right] + \frac{1}{2} \left[ (\bar{G}^{n+1}_{i,j,k+1/2} - \bar{G}^{n+1}_{i,j,k-1/2}) + (\bar{G}^n_{i,j,k+1/2} - \bar{G}^n_{i,j,k-1/2}) \right] + \frac{\Omega}{2} \left[ -W^{n+1}_{i,j,k} - W^n_{i,j,k} \right] = 0 \tag{3.36}
\]

The future time \((n+1)\) terms can then be linearized using a Taylor series expansion. For example, the term \( \bar{E}^{n+1}_{i+1/2,j,k} \) is linearized as follows by neglecting higher order terms,

\[
\bar{E}^{n+1}_{i+1/2,j,k} = \bar{E}^n_{i+1/2,j,k} + \left( \frac{\partial \bar{E}}{\partial V} \right)^n_{i+1/2,j,k} \Delta V^{n+1}_{i+1/2,j,k} \tag{3.37}
\]

where \( \Delta V^{n+1} = V^{n+1} - V^n \). The flux Jacobian term can then be split as

\[
\left( \frac{\partial \bar{E}}{\partial V} \right)^n_{i+1/2,j,k} \Delta V^{n+1}_{i+1/2,j,k} = [A^+] \Delta V^{n+1}_{i,j,k} + [A^-] \Delta V^{n+1}_{i+1,j,k} \tag{3.38}
\]

where

\[
[A^+] = \frac{\partial \bar{E}_{i+1/2,j,k}}{\partial V_{i,j,k}} , \quad [A^-] = \frac{\partial \bar{E}_{i+1/2,j,k}}{\partial V_{i+1,j,k}} \tag{3.39}
\]
Similarly, for $\bar{E}_{i-1/2,j,k}^{n+1}$:

$$\bar{E}_{i-1/2,j,k}^{n+1} = \bar{E}_{i-1/2,j,k}^n + \left( \frac{\partial \bar{E}}{\partial V} \right)_{i-1/2,j,k}^n \Delta V_{i-1/2,j,k}^{n+1} \quad (3.40)$$

$$\left( \frac{\partial \bar{E}}{\partial V} \right)_{i-1/2,j,k}^n \Delta V_{i-1/2,j,k}^{n+1} = [B^+] \Delta V_{i-1,j,k}^{n+1} + [B^-] \Delta V_{i,j,k}^{n+1} \tag{3.41}$$

$$[B^+] = \frac{\partial \bar{E}_{i-1/2,j,k}}{\partial V_{i-1,j,k}}, \quad [B^-] = \frac{\partial \bar{E}_{i-1/2,j,k}}{\partial V_{i,j,k}} \quad (3.42)$$

Carrying out this same procedure for the $\bar{F}$ and $\bar{G}$ in Eq. 3.36 results in additional split jacobians:

$$[C^+] = \frac{\partial \bar{F}_{i,j+1/2,k}}{\partial V_{i,j,k}}, \quad [C^-] = \frac{\partial \bar{F}_{i,j+1/2,k}}{\partial V_{i,j,k+1}}$$

$$[D^+] = \frac{\partial \bar{F}_{i,j-1/2,k}}{\partial V_{i-1,j,k}}, \quad [D^-] = \frac{\partial \bar{F}_{i,j-1/2,k}}{\partial V_{i,j,k}}$$

$$[E^+] = \frac{\partial \bar{G}_{i,j,k+1/2}}{\partial V_{i,j,k}}, \quad [E^-] = \frac{\partial \bar{G}_{i,j,k+1/2}}{\partial V_{i,j,k+1}}$$

$$[F^+] = \frac{\partial \bar{G}_{i,j,k-1/2}}{\partial V_{i,j,k-1}}, \quad [F^-] = \frac{\partial \bar{G}_{i,j,k-1/2}}{\partial V_{i,j,k}} \quad (3.43)$$

The $(n+1)$ terms for the conservative variables and the source terms are also linearized in a similar fashion,

$$U_{i,j,k}^{n+1} = U_{i,j,k}^n + \left( \frac{\partial U}{\partial V} \right)_{i,j,k}^n \Delta V_{i,j,k}^{n+1} \quad (3.44)$$

$$W_{i,j,k}^{n+1} = W_{i,j,k}^n + \left( \frac{\partial W}{\partial V} \right)_{i,j,k}^n \Delta W_{i,j,k}^{n+1} \quad (3.45)$$

The linearized terms are then substituted back into Eq. 3.36 to obtain

$$-R_{i,j,k}^n = \left[ \frac{\Omega}{\Delta t} \frac{\partial U}{\partial V} + \tilde{A} - \frac{\Omega}{2} \frac{\partial W}{\partial V} \right]_{i,j,k}^n \Delta V_{i,j,k}^{n+1} + \bar{B} \Delta V_{i+1,j,k}^{n+1} + \bar{C} \Delta V_{i-1,j,k}^{n+1} + \
\bar{D} \Delta V_{i,j+1,k}^{n+1} + \bar{E} \Delta V_{i,j-1,k}^{n+1} + \bar{F} \Delta V_{i,j,k+1}^{n+1} + \bar{G} \Delta V_{i,j,k-1}^{n+1} \quad (3.46)$$

where $\tilde{A} - \bar{G}$ are newly defined block matrices obtained by grouping. This results in a matrix system of the form $\tilde{A}\tilde{x} = \tilde{b}$, where $\tilde{x}$ is an ordering of the vector $\Delta V_{i,j,k}^{n+1}$, and $\tilde{b} = -R^n$. Instead of inverting the coefficient matrix $\tilde{A}$, an approximation to $\tilde{A} \approx \tilde{M}$ can be found by using an
Incomplete Lower-Upper (ILU) factorization. This new matrix $\hat{M}$ is relatively easy and cheap to assemble, and allows for faster convergence of the solution. In general, it can be assembled using the block diagonal $D$, and the lower ($\hat{L}$) and upper ($\hat{U}$) triangular matrices as follows

$$\hat{M} = (D + \hat{L})(D)^{-1}(D + \hat{U})$$

(3.47)

Using this definition for the formulation of the present problem given by Eq. 3.46, the lower and upper matrices are

$$\hat{L} = \tilde{C} + \tilde{E} + \tilde{G}$$

(3.48)

$$\hat{U} = \tilde{B} + \tilde{D} + \tilde{F}$$

(3.49)

and therefore, the $\hat{M}$ term is obtained from Eq. 3.47 as

$$\hat{M} = (D + \tilde{C} + \tilde{E} + \tilde{G})(D)^{-1}(D + \tilde{B} + \tilde{D} + \tilde{F})$$

(3.50)

where $D$ is found recursively from

$$D = \left[ \frac{1}{\Delta t} \frac{\partial U}{\partial V} + \hat{A} - \frac{1}{2} \frac{\partial W}{\partial V} \right] - \hat{B}(D)^{-1}\tilde{C} - \hat{D}(D)^{-1}\tilde{E} - \hat{F}(D)^{-1}\tilde{G}$$

(3.51)

The system $\hat{M}\Delta V_{n+1} = -R^n$ is then solved in two steps as follows,

$$(D + \tilde{C} + \tilde{E} + \tilde{G})\Delta V_{i}^{n+1/2} = -R^n$$

(3.52)

$$(D + \tilde{B} + \tilde{D} + \tilde{F})\Delta V_{i}^{n+1} = D\Delta V_{i}^{n+1/2}$$

(3.53)

Finally, the vector of primitive variables is updated:

$$V^{n+1} = V^n + \Delta V^{n+1}$$

(3.54)

A subiteration procedure [25] was also used between time steps in order to enhance convergence within each iteration. In this work, 6 subiterations per time step were used for unsteady problems.
Chapter 4

Simulations of Mach 6 Wake Flow

In this chapter, the performance of the LES/RANS methodology is assessed for separated wake flow problems. Data obtained from a series of experiments performed at the CUBRC LENS facility is used to evaluate the performance of the hybrid LES/RANS approach, and comparisons are made with RANS, and with DES results from [5] (provided by Dr. Barnhardt). First, details regarding the experiment, instrumentation and test conditions are presented. This is followed by a brief description of the computational approach to simulating this problem. Finally, the results of simulations for two different flow conditions are presented and compared with experimental data. The results for a high Reynolds number, fully turbulent flow are discussed first, followed by a discussion of a nominally transitional flow.

4.1 Experimental Details

To validate our CFD code, data presented in [5] [44] was used, which has been previously compared to DES simulations by Barnhardt, Candler and MacLean [5]. The experiments were carried out in the LENS 48” shock tunnel at the CUBRC facilities using a 10-inch-diameter model of a spherical re-entry capsule. The model’s geometry is smooth, and it is representative of the dimensions of the Orion MPCV at the time of the experiment. The dimensions of the model are presented in Figure 4.1, and additional information, including the sting dimensions can be found in [5]. Preliminary studies were carried out to optimize the model’s size and sting configuration, with particular emphasis on having ample steady-state test time [43]. The model’s instrumentation consisted of 35 PCB pressure sensors and 39 heat transfer gauges, with only 7 pressure gauges and 6 heat transfer gauges on the capsule’s forebody. All the heat transfer gauges installed on the backshell were 0.125” thin film platinum resistance elements, and four coaxial thermocouples and two 0.040” thin film gauges were used on the forebody [5] [44]. Thin film gauges were best suited for this study due to their small thermal inertia and
high frequency response. Most of the instrumentation was focused on the model’s backshell as this was the main region of interest during this study. Figure 4.2 shows the distribution of pressure and heat transfer gauges used for the experiments, and additional details can be found in the references. In this investigation, we follow the same instrumentation numbering convention introduced in [5].

Figure 4.1: Dimensions (in inches) of Orion MPCV model used in CUBRC experiments

Testing was carried out with air as the test gas at an angle of attack of 28 degrees, which corresponded to the capsule’s maximum lift-to-drag ratio, and using different sting installations which included a split sting, a diamond cross-section sting, and a round cross-section sting. However, only the round sting configuration is considered in these simulations. Finally, different Reynolds numbers ranging from fully laminar to turbulent flow along the windside afterbody were tested, but this work focused on the highest Reynolds number run, labeled "Run 2" to be consistent with the references [5]. This highest Reynolds number presents an excellent test case for validating the turbulence model. A lower (transitional) Reynolds number case is also studied for comparison with the CFD model, which is referred to as "Run 3". The test conditions for the two cases considered are presented in Table 4.1.
Figure 4.2: Location of model instrumentation: a) Pressure gauges on the afterbody, b) pressure gauges on the forebody, c) heat transfer gauges on the afterbody, d) heat transfer gauges on the forebody.

Table 4.1: CUBRC experiments test conditions

<table>
<thead>
<tr>
<th></th>
<th>Run 2 - Turbulent</th>
<th>Run 3 - Transitional</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re_D$</td>
<td>$11 \times 10^6$</td>
<td>$6 \times 10^6$</td>
</tr>
<tr>
<td>$M_\infty$</td>
<td>6.41</td>
<td>6.43</td>
</tr>
<tr>
<td>$\rho_\infty$(kg/m$^3$)</td>
<td>0.19252</td>
<td>0.11229</td>
</tr>
<tr>
<td>$U_\infty$(m/s)</td>
<td>1102.46</td>
<td>1106.85</td>
</tr>
<tr>
<td>$T_\infty$(K)</td>
<td>73.63</td>
<td>73.76</td>
</tr>
<tr>
<td>$T_{wall}$(K)</td>
<td>295.56</td>
<td>292.78</td>
</tr>
</tbody>
</table>
4.2 Computational Approach

For parallel communication, REACTMB uses MPI message passing. Additionally, inviscid fluxes for these simulations are extended to higher order by the PPM method, and the vorticity-divergence function of Ducros [12] is used to extend the scheme to fourth order accuracy in smooth regions. When the Ducros switch is implemented, the scheme is referred to as a low dissipation (LD) scheme. Air was treated as a calorically perfect gas since the total temperature (∼680 K for Run 2) was not high enough to cause any vibrational excitation or dissociation of the gas.

A three dimensional shock-adjusted grid provided by Barnhardt, Candler and MacLean [5] was used. The grid is made of 9.7 million cells, and a large number of cells were focused in the near wake region where the typical cell width is approximately 1% of the capsule diameter. The surface grid is made of approximately 900,000 cells on the capsule and sting surfaces. The outer inflow boundary was shock fitted, and the computational domain extends approximately 3 capsule diameters downstream of the base region. Slices of the grid at the symmetry plane are shown in Figure 4.3.

A supersonic inlet boundary condition was applied at the inflow (shock-fitted) surface, an extrapolation boundary condition was applied at the exit plane, and the wall was modeled as a viscous isothermal wall due to the short duration of the experiments (10-20 ms). All runs were performed on the same 3D grid described, and the shock always remained within the inflow surface. Simulations were started by computing a steady RANS solution first using Menter’s BSL model. For the LES/RANS simulations, all solutions were started from the converged RANS results, and they were run for approximately 5-8 flow-through times (based on capsule diameter and freestream velocity) to ensure that the solution had reached a statistically invariant state. This was monitored closely by observing the response at all gauge locations and ensuring that the pressure (and heat transfer) predictions had reached a statistically steady behavior. Finally statistics were collected for an additional 5 flow-through times.

4.3 Fully Turbulent Flow Results

This high Reynolds number case was shown to be a good candidate for evaluating high fidelity turbulence models in [5]. This case presents a unique set of challenges for CFD codes such as the large range of turbulent scales present in the flow, ranging from the thin boundary layer structures to the large eddies present in the wake and recirculation region. Other challenges include capturing the unsteady shear layer which directly affects the size and shape of the recirculation region, and resolving the different frequencies associated with flow structures in the separated region. Using this test case, different numerical aspects are addressed such as the
Figure 4.3: Symmetry plane slices of computational grid used for all simulations in this chapter. A full slice of the domain is shown on the right, and a detail view of the near wake region is shown on the left image.
effects of using a low-dissipation scheme, modifications to the blending function, and filtering of CFD results. Comparisons are made between RANS (BSL), LES/RANS, and DES results from [5].

4.3.1 Low Dissipation PPM scheme vs. PPM

In this work, inviscid fluxes were evaluated using the Piecewise Parabolic Method (PPM). However, when working with high fidelity turbulence models it is important to implement a low dissipation scheme in order to avoid dissipating turbulent structures of the same order as the grid scale (and sometimes greater). The present low dissipation scheme uses the well-known function of Ducros [12], and when doing so, we refer to this method as Low Dissipation PPM (LDPPM) scheme. Figure 4.4 shows a comparison of instantaneous temperature contours at the symmetry plane obtained using PPM and LDPPM schemes. The figure also highlights the main features typical of hypersonic base flows: a strong bow shock ahead of the capsule, attached flow along the windside portion of the afterbody, an unsteady shear layer extending from the leeside shoulder separating the outer flow from a large recirculation region, and the periodic shedding of vortices caused by rolling up of the shear layer. A small recirculation region, and a secondary shock, are also seen at the windside junction of the sting and the capsule’s base. Even though the figure only provides a qualitative comparison between the hybrid methods, it is evident that the low dissipation scheme is able to resolve smaller turbulent structures within the wake and near the sting. However, quantitative comparisons between the two methods will be made when comparing pressure and heat flux values with experimental data in a later section.

4.3.2 LES/RANS Blending Function

Early in the study, it was found that the LES/RANS results were significantly underpredicting heat flux levels along the windside afterbody when compared to RANS results and the experimental data. Figure 4.5 shows the heat flux predictions by the RANS and LES/RANS (LDPPM) models for the afterbody gauges along the windside centerline. The “original blending” results were obtained using the blending function as described in section 2.7, and the “modified” blending function formulation is described in 2.7.1. Gauge 51 represents the state of the flow close to the forebody shoulder where the flow is laminar and therefore heat flux levels are relatively low. Moving towards the rear of the capsule, heat flux levels show a gradual increase due to the boundary layer transitioning to turbulent. At gauge 48, the flow has reached a fully turbulent state, and the RANS model predicts the heat flux levels with very good accuracy. Because we did not implement a transition model in this work, the RANS model predicts turbulent heating levels along the entirety of the ray.

For an attached boundary layer, it would be expected that the LDPPM model predictions
should closely resemble the RANS results. Additionally, similar cases found in the literature have shown very good results even with just RANS models along the windside of the capsule [30] [5] [9]. Closer inspection of the model’s behavior showed that the resolution of the grid near the solid boundaries was not fine enough for an LES method. In fact, the grid used for this study was originally developed for DES simulations, in which the entirety of the boundary layer is modeled using a RANS model, and the grid spacing near walls is kept coarse enough so that the model does not transition to LES until outside the boundary layer. However, as described in section 2.7, the current approach is designed to transition within the boundary layer, thus allowing the LES model to resolve outer layer turbulence scales. By implementing the “modified” blending function proposed in 2.7.1, much improvement was seen in the response of the hybrid model as shown in Figure 4.5 (left), where the predictions obtained with the blending correction produced results much closer to the RANS response.
Figure 4.5: Computed heat flux distribution along gauges on the leeside centerline on model's afterbody (left), and computed eddy viscosity and blending function at gauge 50 location using different versions of blending function (right).
4.3.3 Pressure and Heat Transfer Comparisons

In this section, direct comparisons are made between CFD results and experimental data. When evaluating these results, the percent error is normalized by the peak pressure or heat transfer value as follows:

\[ X(\% \text{error}) = \frac{X_{CUBRC} - X_{CFD}}{X_{CUBRC,stag}} \times 100 \]  

(4.1)

where \( X \) represents the quantity of interest, and \( X_{CUBRC,stag} \) is the experimental forebody stagnation point value. Additionally, all error bars shown in the figures represent one standard deviation based on the time variance of the signal. Thus, the error bars do not represent any measure of experimental uncertainty, but they do provide an idea of the unsteadiness of the flow at each gauge location. The LES/RANS results presented in the remainder of the chapter use the modified blending function described in section 2.7.1.

Pressure predictions by the different models all showed reasonable agreement with experiment at most heatshield locations as shown in Figure 4.6. The pressure at gauge 1 is approximately 2.2 MPa and it is located very near the capsule’s stagnation point. As the flow expands around the forebody and towards the leeside, all the models do a very good job of predicting the rapid decrease in pressure. However, larger differences were found along the backshell gauges, and Figure 4.7 presents a direct comparison of pressure results obtained using the different turbulence models considered. Gauges 28 and 8-11 were inoperable during the test and are not shown. As expected, the pressures along each ray of gauges is relatively constant inside the separated region due to enhanced turbulent mixing. Also, pressure results are not too sensitive to the use of the low-dissipation switch, as both PPM and LDPPM show very similar pressure predictions. However, some differences are noticeable between DES and LES/RANS results, where the DES results show better agreement (in general) with the experiment in the recirculation region. Still, all models (including RANS) are able to predict pressures which are within 1% of the peak pressure value. Along the attached boundary layer (gauges 31-35), all models show very similar results and are very close to the experiment, with the exception of gauges 31 and 35, where the gauges appear to be outliers due to the good performance of other surrounding gauges [5].
Figure 4.6: Forebody pressure comparisons between CUBRC experiment, RANS, LES/RANS and DES ([5]) for Run 2 conditions.
Figure 4.7: Afterbody pressure comparisons between CUBRC experiment, RANS, LES/RANS and DES ([5]) for Run 2 conditions.
Modeling heat transfer presents a greater challenge than wall pressure. Figure 4.8 shows results for heat flux levels predicted at each of the forebody sensor locations. All models significantly overpredict gauge 36 which is located at the windside shoulder where the flow expands rapidly as it travels to the backshell of the capsule. MacLean et al. noted in [44] that the adjacent gauge on the backshell of the capsule always remains laminar, which would suggest that the flow around this shoulder could be laminar. However, laminar computations were not carried out in this study to confirm this. Additionally, all models tend to underpredict the heat flux closest to the stagnation region (gauges 37 and 38), which Barnhardt, Candler and MacLean point out is a recurring problem for stagnation point heat transfer in high Reynolds number flows [5] [44]. In this stagnation region LES/RANS consistently predicts higher heat fluxes than DES. At the location of gauge 38, the LES/RANS results closely match those produced by just the RANS BSL model, which suggests that the difference between the LES/RANS schemes and DES at this location are produced by the different RANS models used (BSL vs. Spalart-Allmaras, respectively). Good agreement is seen between all models for gauges 39-41, where the flow appears to be fully turbulent.

Figure 4.8: Predicted heat fluxes at forebody heat gauge locations using RANS, LES/RANS and DES ([5]) for Run 2 conditions.
In Figure 4.9, a comparison between the experimental data and results obtained by different models is shown for the heat fluxes on the capsule’s backshell. Note that the ordinate of each plot may be different in order to present the data more clearly. Along attached flow rays (gauges 47-51, 70-74) all models predict almost the same heating rates at each location, due to the RANS component being active in these regions for the hybrid models. In addition, they all are in very close agreement to the experiment with the exception of the windside centerline gauges. In this centerline ray, all models overpredict gauges 49-51 since the boundary layer is transitioning to turbulence and no transition model has been implemented. The differences between all the models (which are in close agreement) and gauge 72 also appear to be a consequence of transition, as suggested by the large unsteadiness in this gauge. MacLean et al. have proposed that thin-film gauges can give a good indication of transition onset when the standard deviation of the signal increases [44], which supports the hypothesis that the flow near gauge 72 is transitional.

As expected, greater differences amongst the models and with the experiment appear along rays in the separated region. Along the leeside centerline ray (gauges 41-46), the RANS model significantly overpredicts heat flux, by up to three times the experimental data at gauge 45. In general, RANS overpredicted heat fluxes throughout the separated region, with the exception of gauges 57 and 61. In Figure 4.10, temperature contours of results obtained using RANS and LES/RANS show that the RANS model predicts wake temperatures that are much higher than the hybrid scheme. In regions close to the base, along the sting, and near the recompression shock, temperature differences of over 100 K are seen between RANS and LES/RANS. The hotter temperatures seen in the recirculation zone result in higher heat transfer predictions in the separated region. Because the higher fidelity methods are able to capture more of the relevant unsteady physics of this wake flow, the temperature distributions are more consistent with the experiment, resulting in more accurate heat transfer predictions.
Figure 4.9: Afterbody heat transfer comparisons between CUBRC experiment, RANS, LES/RANS and DES ([5]) for Run 2 conditions.
Figure 4.10: Temperature contours at symmetry plane showing differences in predicted wake temperatures. a) Steady RANS (BSL) contours, b) Time-averaged LES/RANS LDPPM contours, c) Instantaneous contours using LES/RANS LDPPM.
The LES/RANS PPM and LDPPM schemes produce very similar results along the separated region, and in general, they are also in close agreement with the experimental data (Figure 4.9). However, most of the differences between these two models, and between the CFD and the experiment, arise at the gauge locations on the conical afterbody closest to the base. For example, at gauge 45 the LDPPM scheme underpredicts the experimental data by 1.5%, while the PPM scheme underpredicts it by 0.65% of the peak heating value. DES also has some difficulties modeling this gauge location, where it overpredicts the mean experimental value by about 1% of the stagnation heating value. At gauge 56, the LDPPM model overpredicts the heat flux value by over 2%, while the PPM scheme and the DES models do a much better job of predicting the response of this gauge.

A more qualitative assessment of the performance of each model can be made by examining the heat flux percent error as shown in Figure 4.11. In this plot, negative values indicate an overprediction of the CFD model and positive values correspond to underpredictions. The error at each thin-film gauge location on the capsule’s forebody is shown for each of the models considered, including the results obtained in [5] using DES. It is clear from this figure that RANS overpredicts most leeside gauges by over 2% of the peak heating value. Also, all hybrid models show similar trends along the windside gauges, which are also consistent with the RANS results. For the most part, the PPM and LDPPM results are very similar throughout the separated region, with the exception of the leeside centerline ray and the gauges located on the rear shoulder, where the PPM scheme shows closer agreement with experiment. The results obtained using DES show the closest agreement with experiment along the leeside centerline ray. Both LES/RANS schemes and the DES model tend to overpredict (by ~1-2%) both gauges located on the base of the model, with the exception of the LDPPM scheme which is able to predict (within 0.3% of peak heating) the heat flux at gauge 47.

To gauge the accuracy of each scheme in different regions around the capsule, a normalized RMS error (NRMSE) was computed at each region $r$:

$$
NRMSE_r = \left[ \frac{1}{n} \sum_{k=1}^{n} \left( \frac{X_{r,CUBRC}^k - X_{CFD}^k}{X_{r,CUBRC}} \right)^2 \right]^{1/2} \times 100
$$

where $n$ represents the number of experimental gauges in region $r$ only, and the index $k$ only includes gauges in $r$. By using this definition, the goal is to isolate the errors in each region by normalizing by an average which is representative of the region considered. A summary of the computed error statistics presented in Table 4.2 for three different regions considered. The analysis divides the capsule into forebody (FB), leeside afterbody (AB-L) and windside.
Figure 4.11: Percent error of heat flux predictions on backshell gauges for Run 2 conditions using a) RANS, b) LES/RANS PPM, c) LES/RANS LDPPM, and d) DES ([5]).
Table 4.2: Normalized RMS error and % error summary for RANS, DES and LDPPM results for Run2 case.

<table>
<thead>
<tr>
<th>Region</th>
<th>RANS</th>
<th>DES ([5])</th>
<th>PPM</th>
<th>LDPPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>FB NRMS error</td>
<td>36</td>
<td>37</td>
<td>30</td>
<td>24</td>
</tr>
<tr>
<td>AB-W NRMS error</td>
<td>53</td>
<td>49</td>
<td>54</td>
<td>53</td>
</tr>
<tr>
<td>AB-L NRMS error</td>
<td>129</td>
<td>38</td>
<td>33</td>
<td>54</td>
</tr>
<tr>
<td>AB-L max</td>
<td>%error</td>
<td>5.33 1.51 1.06 2.39</td>
<td></td>
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</tr>
</tbody>
</table>

afterbody (AB-W) to assess the performance of each model in each of these regions individually. Note that the leeside afterbody region corresponds to nominally separated flow and the windside afterbody to attached flow. Referring to the gauge locations shown in Figure 4.2, the forebody gauges include gauges 36-41, the windside afterbody gauges are 47-51 and 70-74, and the remaining are considered the leeside afterbody gauges (for the purposes of this analysis). These comparisons show that the average error for all models on the forebody is \( \sim 30\% \), and along the backshell windside gauges \( \sim 50\% \). However, these errors are mostly due to the lack of a transition model. Because the RANS model is active in these regions for the hybrid schemes, the differences between all models are small. Recall that the original formulation of the blending between RANS and LES avoids treating the entire boundary layer in attached flows with purely RANS, but as discussed in section 4.3.2, the modifications to the blending mechanism resulted in most of the boundary layer to be treated as RANS (similar to DES). In terms of average percent error in the separated (leeside) region, the RANS results show a much larger average error (129%) as compared to the hybrid schemes (\( \sim 30-50\% \)). The performance of the PPM scheme and DES are very comparable in the leeside region with an average error of \( \sim 35\% \), while the LDPPM results are also very good (54%). Finally, Table 4.2 also compares the maximum error (as defined in Eq. 4.1) found in the heat flux predictions for the afterbody leeside gauges. In general, the worst disagreement between the high fidelity models and experiment was less than 2.5%, while RANS results are off by up to 5% of peak heating in the separated region. Overall, these results demonstrate the much improved accuracy obtained by these hybrid methods over conventional RANS models, and highlight the good performance of the LES/RANS turbulence model as compared to the experiment and DES.

### 4.3.4 Time History Comparisons

To assess the ability of this hybrid method to capture the unsteady characteristics of the flow, a direct comparison between time traces of selected heat transfer gauges along the leeside...
centerline and CFD results was made. The frequency at which data could be collected in the experiment was much smaller than the time step used in our simulations ($\sim 1 \times 10^{-7}$), therefore, it was necessary to filter out the dense CFD results to match the experimental frequencies. To do so in the most physically-accurate manner possible, the behavior of each thin film gauge was modeled by using a material response code and introducing the same physical limitations present when acquiring experimental data.

The Charring Ablator Response (CHAR) code developed by Amar, Calvert and Kirk [3] was used. CHAR is a multi-dimensional thermal material response code used for solving ablating and non-ablating TPS problems, as well as direct and indirect heat transfer problems. It solves problems on structured or unstructured grids using a Galerkin Finite Element Method discretization, and it can operate in serial or parallel operation. For the present purposes, CHAR was used to solve a direct 1-D heat conduction problem to model the response of a 1/8” thick pyrex substrate such as those used in the experimental heat gauges. This was accomplished (at each gauge location) by using the heat flux CFD results as a boundary condition to drive the problem. By doing so, the time-temperature history at the surface of the pyrex substrate was obtained at the same frequency as the CFD results used. This step simulates the fact that in reality, heat transfer gauges cannot measure heat flux directly, and instead, temperature traces are obtained at each gauge and a 1-D numerical integration is performed (as a post-processing step) to obtain heat flux. To introduce the frequency at which gauges are able to obtain temperature data points, the surface temperature history obtained from CHAR was filtered to match the experimental time step (0.24 ms). Finally, using the filtered temperature traces, the numerical technique by Schultz and Jones [55] was used to recover heat flux time traces, where the heat flux at a particular time $t_m$ is obtained from:

$$q_w(t_m) = \frac{\sqrt{\rho c k}}{\sqrt{\pi}} \sum_{i=1}^{m} \frac{2(T_i - T_{i-1})}{\sqrt{t_m - t_i} + \sqrt{t_m - t_{i-1}}}$$

where $T_i$ is the temperature at the discrete data point $i$, corresponding to time $t_i$. In addition, this procedure assumes constant material properties ($\rho, c, k$).

For this filtering procedure, a CFD solution using LES/RANS LDPPM for Run 2 conditions, which was carried out for a time period comparable to the experiment (40 flow times), was used as input for CHAR. Also, a 1-D grid of 100 cells with geometric clustering on the surface of the pyrex slab was used, which a preliminary grid study showed to be converged for this problem. Only gauges 42-26 which are located along the afterbody leeside centerline were considered. The material properties for pyrex were obtained from [10] and they were approximated to be constant due to the short duration of the experiment. The values used for density, thermal conductivity and specific heat capacity were 2333 kg/m$^3$, 1.146 W/m-K, and 840 J/kg-K, respectively.
Results from the material thermal response analysis showed that the temperatures throughout the pyrex substrate remained within one degree of the wall temperature, thus confirming that using an input heat flux which is invariant with wall temperature is a good assumption.

A comparison of the “raw” signal obtained directly from the CFD results and the filtered time trace for gauge 45 is presented in Figure 4.12. For clarity, only ~20 flow times are shown in the comparison, but the figure clearly shows how the filtered signal is still a very good representation of the original transient data, and major low frequency variations of the signal are captured. Furthermore, the filtered signal is unable to capture the high frequency events computed at the gauge location, which also represents the physical limitation of heat transfer gauges used in the experiment. In Figure 4.13, the filtered results for the ray of gauges along the leeside centerline are compared to experimental time traces, and DES results from [5] for direct comparison. Note that only the LES/RANS LDPPM results in the figure have been filtered through the procedure described. In addition, the standard deviation of each time trace was computed for both turbulence models, and they are presented as a fraction of the experimental standard deviation for each gauge in Figure 4.13. On these plots, the “time” axis does not represent a common physical time, but comparing these traces allows for further evaluation of the scheme’s temporal accuracy, and its ability to resolve similar frequencies, trends and amplitudes as those recorded during the experiment. The LES/RANS results on gauge 42 show a clear low frequency variation in the heat flux with a period of approximately 5-10 flow times, which closely resembles the variations observed in the experimental signal. Because of its proximity to the leeside shoulder, where the shear layer initially separates, the heat flux at gauge 42 is particularly sensitive to the unsteady motion of the shear layer. On the other hand, DES results of gauge 42 fail to capture this low frequency, high amplitude content. Barnhardt, Candler and MacLean did, however, show in their study that significant improvements are obtained using a low dissipation scheme for this gauge [5], which explains why the LDPPM scheme is able to perform better at this gauge. The standard deviation of the signal computed with LES/RANS for gauge 42 is 1.24 times the experimental value, highlighting the model’s ability to resolve a very similar level of unsteadiness as seen in the experiment. Closer to the base, the LES/RANS model tends to underpredict mean heat flux levels (gauges 43 and 44), and both LES/RANS and DES underpredict the standard deviation of the time traces. However, at gauge 45, LES/RANS results show very similar amplitudes and frequencies as those seen in the experiment and those obtained by DES. Finally, at the base of the capsule (gauge 46), both DES and LES/RANS tend to overpredict mean heat flux levels and show larger spikes than those recorded during the experiment. Despite the large degree of unsteadiness of this problem, these results demonstrate that the hybrid Low Dissipation LES/RANS scheme is able to capture, with good accuracy; most transient events seen in the experiment.
4.3.5 Time-Averaging

All the time-averaged results presented so far were averaged over a length of five characteristic flow times. However, some heat flux time traces presented in Figure 4.13 show a very low frequency variation of the signal, which could have resulted in inaccurate time-averaged results. For example, the transient signal of gauge 42 contains a low frequency variation with a period of approximately 5-10 flow times, which indicates that time-averaging over 5 flow times was not appropriate for this gauge. Travin, Shur, Strelets and Spalart [63] also warn about the danger of looking at “only one or a few shedding cycles” when examining their results using DES around a circular cylinder. To examine the effect of time-averaging these results over longer time periods, the simulation was run for a length of time comparable to the experiment (∼ 40 flow times), and heat transfer time averages were computed over different time periods for the gauges along the backshell leeside centerline. The results are shown in Figure 4.14 and Figure 4.15. It is evident that the time-averaged heat flux had “converged” after only 5 flow times for most gauges on the backshell, and most of the change observed was localized to the gauges along the centerline in the separated region. In general, the results averaged over 40 flow times match the experimental data more closely as expected. In particular, results for gauges 42 and 45 saw a good deal of improvement, where the percent error improved by a factor of 2 for gauge 42, and from 1.5% to 1% of peak heating for gauge 45. These findings suggest that, for the most part, the comparisons shown thus far using time-averaged data over only 5 characteristic flow times are “converged” for the purposes of this study, with the exception of gauges along the leeside centerline of the
Figure 4.13: Evolution of heat flux levels with time at different leeside centerline heat transfer gauges for Run 2 conditions.
capsule’s backshell (gauges 41-46), where some change was seen when time-averaging over the entire length of the experiment.

Figure 4.14: Effect of time-averaging heat flux predictions over different time spans for backshell gauges on leeside centerline using LES/RANS LDPPM for Run 2 conditions.

Figure 4.15: Heat flux percent error at all backshell heat transfer gauges obtained using LES/RANS LDPPM results time-averaged over 5 flow times (left) and 40 flow times (right).
4.4 Transitional Flow Results

A second case, which is representative of a nominally transitional Reynolds number was considered for additional validation of the LES/RANS LDPPM model and CFD practices. The time-averaged results presented have been averaged over 5 characteristic flow times. In terms of pressure comparisons, trends very similar to those seen in the high Reynolds number case were observed. Figure 4.16 and Figure 4.17 show pressure comparisons between the experiment and the different turbulence models in the forebody and afterbody of the capsule, respectively. All models produce similar results in the forebody, all in very good agreement with the experiment. Along the windside gauges in the capsule’s backshell, essentially identical pressure values were predicted by RANS, DES and LES/RANS, and slight overpredictions at gauges 35 and 31 are once again evident. In the separated backshell region, some differences between the turbulence models were found. DES results follow the experimental data more closely, whereas RANS predictions tend to underpredict pressure and LES/RANS slightly overpredicts pressure. In general though, pressure predictions within 1% of the experimental stagnation pressure were obtained with all three turbulence models.

![Figure 4.16: Forebody pressure comparisons between CUBRC experiment, RANS, LES/RANS and DES ([5]) for Run 3 conditions.](image-url)
Figure 4.17: Afterbody pressure comparisons between CUBRC experiment, RANS, LES/RANS and DES ([5]) for Run 3 conditions.
Heat flux comparisons at forebody gauge locations are shown in Figure 4.18. A significant overprediction of heat transfer by all models is evident at gauge 36, where the flow remains laminar as it turns around the shoulder. Similar discrepancies in heat transfer as those seen in the Run2 results are seen in the stagnation region for all models. Traveling along the forebody centerline towards the leeside shoulder, LES/RANS and RANS results are in close agreement with each other and with the experimental data, whereas DES tends to underpredict heat flux at these locations by up to 30% of the peak heating value.

Backshell heat flux comparisons for this transitional flow are presented in Figure 4.19. As expected, the RANS, DES and LES/RANS models predict very conservative heat flux values along the windside where the flow is attached and still has not transitioned to a fully turbulent state. Excellent agreement is seen between all CFD models and the experiment along the rays closest to the separation line (gauges 67-69). Overall, trends very similar to the previous fully turbulent (Run 2) results are evident for the LDPPM results. Unlike the DES predictions which, calculate an upper bound for heat flux for this transitional flow, the LES/RANS results show excellent agreement with experiment for gauges inside the recirculation zone (gauges 42-45, 52-55, 56-59, 60-63). In addition, LES/RANS predictions along the leeside centerline are in very good agreement with experiment. However, the discussion in section 4.3.5 suggests that the results along these gauges might not be entirely converged, and running this simulation further could result in closer agreement with the experimental data. Both DES and LES/RANS models once again show a tendency to overpredict the heat transfer rates at the base of the capsule. Except for gauges located in attached flow regions, the RANS results overpredict (by up to 6% of the stagnation value in some cases) heat flux levels throughout the separated flow region.
Figure 4.18: Predicted heat fluxes at forebody heat gauge locations using RANS, LES/RANS and DES ([5]) for Run 3 conditions.
Figure 4.19: Afterbody heat flux comparisons between CUBRC experiment, RANS, LES/RANS and DES ([5]) for Run 3 conditions.
Table 4.3: Normalized RMS error and % error summary for RANS, DES and LDPPM results for Run3 case.

<table>
<thead>
<tr>
<th>Region</th>
<th>RANS</th>
<th>DES ([5])</th>
<th>LDPPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>FB NRMS error</td>
<td>33</td>
<td>34</td>
<td>26</td>
</tr>
<tr>
<td>AB-W NRMS error</td>
<td>100</td>
<td>87</td>
<td>101</td>
</tr>
<tr>
<td>AB-L NRMS error</td>
<td>156</td>
<td>93</td>
<td>66</td>
</tr>
<tr>
<td>AB-L max</td>
<td>[%error]</td>
<td>6.06</td>
<td>4.04</td>
</tr>
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</table>

Table 4.3 presents a similar analysis of error statistics as the one presented in section 4.3.3 for the fully turbulent case. Once again, the statistics are computed at different regions of the capsule: forebody (FB), afterbody windside (AB-W), and afterbody leeside (AB-L). In general, the normalized RMS results follow similar trends as those seen for the high Reynolds number case. All three schemes show NRMS errors of ~30% in the forebody region, and on the order of 100% on the attached windside afterbody. Naturally, since the Reynolds number is not high enough to cause the flow to transition entirely along the windside, the errors are larger than those for the higher Re case. However, no advantage of using a higher fidelity scheme is evident over the RANS model, as expected. In the separated region, the hybrid schemes show much improvement once again over RANS. The RANS results show errors of up to 6% of the forebody peak heating, where DES and LDPPM results have maximum error magnitudes of approximately 4% and 2%, respectively. In fact, these results also highlight the improvement in performance of the hybrid LDPPM scheme over DES for this particular run. The lowest NRMS error in the separated region was obtained with our LES/RANS scheme (70%), followed by DES (90%). Finally, the LDPPM integrated error is approximately 1/3 of that obtained using the RANS model in the separated backshell region. In the end, the findings presented for the two different Reynolds numbers considered demonstrate the consistency of our numerical methods and best practices to simulate these types of wake flows with very good spatial and temporal accuracy, and highlight the improvements possible over conventional RANS models for predicting aerodynamic heating of re-entry vehicles.
Chapter 5

Verification and Application for Flows in Thermal and Chemical Nonequilibrium

In this chapter, the recent implementation of thermal nonequilibrium capabilities to REACTMB, and the addition of the Park 1985 chemistry model for air are verified by performing a code-to-code comparison with the established NASA code DPLR [69]. DPLR is a 3D nonequilibrium finite volume Navier-Stokes solver based on the data parallel line relaxation method of Wright, Candler and Bose [68], which has been heavily validated and verified for nonequilibrium hypersonic problems. The two-dimensional flow around a half-cylinder is considered for the verification study taking advantage of the simple geometry, and because historically such flows have been studied in great detail for thermochemical nonequilibrium cases. Finally, a more realistic 3D flow around a spherical capsule at a high Reynolds number is used as a demonstration of the capabilities of the code for simulating nonequilibrium cases using the high fidelity turbulence model. In addition, the study also serves to investigate, in a qualitative sense, the differences between a RANS result and an LES/RANS solution of flows in thermal and chemical nonequilibrium.

5.1 2D Flow Around a Cylinder

The full Navier Stokes equations for a laminar flow around a half-cylinder (1 meter radius) in full thermochemical nonequilibrium are solved in this section. The freestream conditions selected for this test case are shown in Table 5.1. These conditions produce a high total enthalpy flow (∼23 MJ/kg) at low density conditions, which results in prominent nonequilibrium flow features. The freestream air composition was specified by the following mass fractions: $Y_{N_2} = 0.78$, $Y_{O_2} = 0.22$, etc.
Table 5.1: Cylinder cases freestream conditions

<p>| | |</p>
<table>
<thead>
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<tbody>
<tr>
<td>$M_\infty$</td>
<td>20.8</td>
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<tr>
<td>$\rho_\infty$ $(kg/m^3)$</td>
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</tr>
<tr>
<td>$U_\infty$ $(m/s)$</td>
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<tr>
<td>$T_\infty$ $(K)$</td>
<td>265</td>
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<tr>
<td>$T_{v\infty}$ $(K)$</td>
<td>265</td>
</tr>
<tr>
<td>$T_{wall}$ $(K)$</td>
<td>1456</td>
</tr>
</tbody>
</table>

$Y_{NO} = Y_N = Y_O = 0$. A supersonic inflow boundary condition was applied at the inflow plane by fixing the pressure, translational/rotational temperature, vibrational temperature, and velocity at their corresponding freestream values. In addition, an extrapolation boundary condition was enforced at outflow planes. A no-slip condition was applied at the walls in order to enforce a viscous wall boundary, and the temperature at the wall was kept constant throughout each simulation. Since experimental results have shown that vibrational temperatures of molecules near walls are very similar to the wall temperature [50], the vibrational temperature at the wall is set equal to the wall temperature. When dealing with finite-rate chemistry, additional wall boundary conditions must also be specified on the state of the chemical process at the wall. In this work, walls are modeled as non-catalytic by setting all species diffusion mass fluxes to be zero at the walls.

A preliminary grid study was carried out by considering three different grids with increasing mesh refinement. The grids were created in Gridgen and then DPLR was used to shock-align each of the grids. The grids used are labeled as “baseline”, “fine” and “very fine”, and they are shown in Figure 5.1. A uniform spacing was used in the circumferential direction, and the baseline, fine and very fine grids had 160, 250 and 350 circumferential cells, respectively. In the wall normal direction, the mesh was clustered near the wall to resolve the viscous layer, and the baseline, fine and very fine grids have 122, 150 and 250 cells, respectively.

The results of the grid sensitivity study are presented in Figure 5.2, where the temperatures, pressure and streamwise velocity are shown along the stagnation streamline. As expected, the finest grid provides the best resolution along the stagnation line. The “very fine” grid is able to resolve the shock discontinuity best, but all three grids show very similar results downstream of the shock. Even though using the finest grid results in longer computing time, this 2D problem converges relatively quick on multiple processors, therefore the “very fine” grid was used for the rest of the study to improve resolution of the shock.
Figure 5.1: 2D cylinder grids used for grid sensitivity study. Left: baseline grid, Center: fine grid, Right: very fine grid.

Figure 5.2: Stagnation line profiles obtained using three different grid resolutions for translational and vibrational temperatures (left), and pressure and streamwise velocity (right).
5.1.1 Code Verification

A second order TVD scheme using the minmod limiting function was used to extend inviscid fluxes to higher order for these results. Preliminary work for this problem showed that the TVD scheme was able to resolve the stagnation line features somewhat better than the PPM scheme. In addition, inviscid fluxes are computed using the LDFSS as described in previous chapters, and the implicit time advancement yields second order temporal accuracy. For this verification study, DPLR was run using the same chemistry model, thermal-nonequilibrium assumptions, and transport properties models as those described in this work. Also, DPLR uses a modified Steger-Warming flux vector splitting for computation of inviscid fluxes, and the spatial order of accuracy was set to second order. Figure 5.3 shows the results obtained using REACTMB and DPLR for flowfield density, pressure, streamwise velocity, translational/rotational temperature and vibrational temperature. Overall, the comparisons show excellent agreement between the two codes. There are slight differences between the density contours very close to the cylinder wall, however, these differences are very isolated near the stagnation region. In general, differences in the stagnation region of supersonic problems on blunt bodies (such as this cylinder) are to be expected. This stagnation region for these types of problems is prone to non-physical instabilities due to the numerical method used, and due to grid alignment and grid stretching. Because the grid resolution is typically not enough to resolve the thin shock wave, these regions are dominated by numerical dissipation instead of physical dissipative effects, which can result in the so-called “carbuncle” instabilities.

There are also slight differences present between the two codes in the magnitudes of vibrational temperatures near the shock, where DPLR results show higher vibrational temperatures as you move away from the centerline in a very thin region near the shock. The agreement between the temperatures predicted by each code can be examined more closely by looking at the results only along the stagnation line and along the outflow boundary as in Figure 5.4. The stagnation line plot shows the classical $T - T_v$ response across a normal shock wave. As the flow is suddenly shocked, the energy in each of the different modes of the air molecules see a sharp increase as well, which manifests itself as jumps in temperatures. In addition, this shocking of the flow also initializes the chemical reactions which lead to the creation of new species. After the initial temperature spike, the translational/rotational and vibrational temperatures begin to relax to post shock values at different rates. The vibrational temperature decreases at a slower rate than the translational temperature, which results in regions where the vibrational temperature is actually higher than the translational temperature. This vibrational relaxation process is more evident as the freestream density is decreased. This can be explained in a physical sense because it takes longer for sufficient molecular collisions to occur to equilibrate the different energy modes. In a modeling sense, this process is governed by the Landau-Teller
component of the vibrational source term in Eq. 2.31. Noting the presence of the species density term in Eq. 2.31, and also the presence of the pressure term (which is proportional to density) in Eq. 2.33, this source term is essentially proportional to the square of density. Therefore, lower density conditions result in a smaller driving source term to restore thermal equilibrium between the translational and vibrational modes. Overall, excellent agreement is seen between the two codes for translational temperature \( T \) along the stagnation line and the outflow plane. The outflow plane profiles for vibrational temperature show some more significant differences though (on the order of 1000 K). The DPLR vibrational energy model tends to predict lower vibrational temperatures at this plane than REACTMB. However, it was later found that DPLR uses different coefficients for the Millikan-White expression (Eq. 2.33) for certain specific reactions, which results in vibrational temperature differences between the two codes. Given the empirical origin and the uncertainties of the constants used for these models though, the differences in vibrational temperatures at the outflow plane between the two codes are not of great concern. In addition, the previous results shown in Figure 5.3 demonstrated good general agreement for vibrational temperatures between the two codes.

Additional comparisons between the two codes are shown in Figure 5.5, where the species mass fractions for molecular nitrogen, nitrous oxide, atomic nitrogen and atomic oxygen are compared. The presence of the strong shock causes all of the molecular oxygen and some of the molecular nitrogen to dissociate. Oxygen dissociates first due to the lower activation energy in the oxygen dissociation reaction. The complete dissociation of oxygen results in the creation of atomic oxygen \( \text{O} \), and allows reactions to proceed to create nitrous oxide \( \text{NO} \). However, most of the NO is only present immediately after the shock, and it quickly dissociates within the shock layer. Overall, the figures show excellent agreement between the two codes. Additionally, the stagnation line and outflow plane species profiles are examined in more detail in Figure 5.6. The solid lines represent results obtained using REACTMB while the dash-dot lines are extracted from DPLR results. The mass fractions are shown in a log scale to obtain better comparisons over the large range of mass fraction values. Along the stagnation line, the shock occurs at approximately 0.16 meters away from the body, where a sudden decrease in \( \text{O}_2 \) mass fractions begins. Molecular oxygen dissociates almost entirely, going from a freestream mass fraction of 0.22 to post-shock levels which are 3 to 4 orders of magnitude smaller. Only about half of the molecular nitrogen dissociates, going from 0.78 mass fraction in the freestream, to approximately 0.4 within the shock layer. NO mass fractions reach a maximum (\(~0.08\)) very close to the shock, and quickly dissociates into N and O within the shock layer. As the temperature drops to wall temperature levels within the boundary layer, the NO mass fraction drops to essentially zero near the wall. Along the outflow boundary, similar trends to the stagnation line profiles are seen. The shock is located about 0.8 meters from the top of the cylinder. The \( \text{N}_2 \) mass fractions remain relatively constant within the shock layer. A sharp increase in atomic oxygen mass...
Figure 5.3: Code-to-code comparisons between REACTMB and DPLR for a) density, b) pressure, c) streamwise velocity, d) translational/rotational temperature, and e) vibrational temperature.
fractions is present near the shock, and it levels out at approximately 0.2 within the shock layer. The gradients of atomic nitrogen are more gradual along the outflow boundary, and the maximum N mass fraction (∼0.3) is found closer to the wall. Finally, the NO mass fraction reaches a maximum right past the shock and continually decreases within the shock layer by approximately 5 orders of magnitude, being essentially zero at the wall. The profiles shown for mass fractions along the stagnation and outflow lines computed with both codes show excellent agreement, and it verifies the implementation of the Park 1985 chemistry model in REACTMB.

5.1.2 Nonequilibrium Effects at Different Altitudes

In this section, the nonequilibrium version of REACTMB is tested under different freestream conditions, corresponding to variations in the altitude (or freestream density). The same freestream conditions, grid and computational approach as those described in the previous section are used for these simulations, however, three different farfield densities are considered: 0.0001, 0.001 and 0.01 kg/m³. The stagnation line profiles for $T$ and $T_v$ are shown in Figure 5.7. The results show more pronounced peaks in both temperatures, and the most significant extent of thermal nonequilibrium, for the lowest density case. As part of the energy is deposited in the vibrational modes, and energy goes into dissociating molecular species, the translational/rotational temperature decreases after the shock. The results clearly show how the higher the density, the quicker
Figure 5.5: Code-to-code comparisons between REACTMB and DPLR species mass fractions for a) $\text{N}_2$, b) NO, c) N, and d) O.
Figure 5.6: Code-to-code comparisons between REACTMB and DPLR species mass fractions along the stagnation line (left) and outflow plane (right).
equilibrium is achieved. For the highest density case (0.01 kg/m$^3$), there is actually only a very small degree of thermal nonequilibrium, followed by very constant post-shock temperatures of approximately 7000 K. In Figure 5.8, the distributions of vibrational temperature are shown for the three densities considered. Again, the results show much higher vibrational temperatures for the lowest density case where vibrational temperatures above 10,000 K are seen, and these higher vibrational temperatures are present about halfway into the shock layer. For the medium density (1E-3 kg/m$^3$), high vibrational temperatures are seen in a very thin region near the shock, but temperatures quickly drop to equilibrium values (about 6000 K). The vibrational temperatures are more evenly distributed for the high density case as the vibrational mode is essentially in thermal equilibrium with the translational/rotational mode throughout the shock layer.

![Figure 5.7: Thermal nonequilibrium effects along stagnation line for three different densities.](image)

Finally, the results of varying freestream density on the resulting mass fraction distributions for N$_2$, N, and NO are shown in Figure 5.9. The contours for O$_2$ and O mass fractions, although not shown, simply show almost complete dissociation of O$_2$, accompanied by a corresponding increase in O mass fractions for all three densities considered. The highest density case shows
the least amount of nitrogen dissociation, especially in off-stagnation line regions. It also shows
the least amount of NO production and it is most noticeable near the shock away from the
stagnation line. The medium density case (1E-3 kg/m³) actually shows more rapid dissociation
of nitrogen than the lowest density case, and N mass fractions of up to 0.3 are present near
the stagnation region for most of the shock layer. On the other hand, the lowest density case
actually shows the greatest presence of NO with mass fractions of up to 10%. In regions further
away from the centerline, where the shock is actually weaker and the post-shock densities are
lower, larger amounts of NO are found due to longer times for the NO dissociation process to
take place. These results highlight the complexity of hypersonic blunt-body flows, for which
there are not always clear trends observed in terms of the flow’s chemical composition with
varying freestream properties.

5.2 3D Flow Around a Spherical Capsule

To test the robustness of REACTMB for a more practical application, a 3D flow around a
re-entry capsule similar to the Orion MPCV is considered with full thermal and chemical
nonequilibrium effects. A grid originally designed for wind-tunnel simulations is used for this
case, however, the geometry is scaled up to flight scale in order to ensure a fully turbulent
flow. Originally, a 29 million cells grid was designed for a 10-inch-diameter model of the Orion
MPCV, for both RANS and LES/RANS simulations. However, it was designed for wind-tunnel
Figure 5.9: Contours of species mass fractions for a) N₂, b) N, and c) NO for the three different densities considered.
conditions for a Mach 8 flow, and in this work the grid was scaled up to a 5m-diameter capsule, which is similar to a full-scale Orion. A great amount of effort was devoted to keeping the cells in the wake region as orthogonal as possible, and small enough to resolve the most energetic eddies in the recirculation zone. The design process was based on the grid shown in Chapter 4 provided by Dr. Barnhardt, and on best practices for the LES/RANS model developed at NC State. The sting was extended about 3 capsule diameters downstream with 248 cells in the streamwise direction along the sting. The capsule geometry contains 172 off-body cells, 320 cells in the circumferential direction, and 210 cells along the backshell streamwise direction. The cells in the wake region have an average cell size of less than 0.5% of the capsule diameter. Figure 5.10 shows symmetry plane slices of the computational domain. It is recognized that this grid may not be realistic due to the incorporation of a sting on a full-scale model, and the grid spacing has not been properly optimized for these conditions, however, these results serve as a first-order test of REACTMB for a separated turbulent flow with nonequilibrium effects.

Figure 5.10: Distribution of mesh cells in the symmetry plane of the domain (right), and detail view of mesh in the near wake region (left).

Freestream conditions from the Fire-II re-entry experiment are used in these simulations since the conditions are enough to cause nonequilibrium phenomena, and the trajectory point selected has been used in the literature to assess the performance of a DES turbulence model [57]. The conditions are listed in Table 5.2. An angle of attack of 18 degrees was used since the grid was designed for this angle of attack, and the freestream air composition was defined
in mass fractions as: $Y_{N_2} = 0.78$, $Y_{O_2} = 0.22$, $Y_{NO} = Y_N = Y_O = 0$. Based on the 5m diameter vehicle, the Reynolds number for this case is approximately $15 \times 10^6$, resulting in a fully turbulent base flow. Steady RANS simulations were carried out using Menter’s BSL model as described in Chapter 2, and unsteady LES/RANS simulations were initialized from these RANS results. Unsteady LES/RANS simulations were run initially for five flow-through times (based on capsule diameter) to clear the solution of initial transients, and statistics were collected for an additional 5 flow times.

In Figure 5.11 the resulting distributions of translational/rotational temperature $T$ are shown for RANS and time-averaged LES/RANS results, and an instantaneous LES/RANS snapshot is also shown. The figure shows the temperature contours at the pitch plane, and at an out-of-plane slice located approximately half a capsule diameter downstream from the base. Compared to the time-averaged LES/RANS result, the RANS model predicts much higher temperatures in the near wake and close to the sting surface, which is consistent with the findings presented in chapter 4. Further downstream, the LES/RANS model predicts a more uniform temperature distribution throughout the flowfield, while the RANS results show more significant temperature variations. In the capsule’s forebody region, both models predict almost identical temperatures as one would expect. The instantaneous snapshot highlights the ability of LES/RANS to capture the smaller temperature fluctuations observed in the wake region and the recirculation zone.

The vibrational temperature distributions obtained with each of the turbulence models are shown in Figure 5.12. As expected, the vibrational temperature is increased significantly within the shock layer as the flow crosses the bow shock. Both the RANS and the LES/RANS models predict forebody vibrational temperatures on the same order as the post-shock translational/rotational temperatures, but slightly lower as expected. However, unlike the translational/rotational temperature, which decreases rapidly as the flow travels around the shoulder and expands, the vibrational energy pool becomes frozen, and vibrational temperatures re-
main at levels close to those found in the shock layer. However, clear differences between the vibrational temperatures predicted by RANS and LES/RANS are seen in the separated region, where RANS predicts vibrational temperatures over 1000 K higher than those seen in the time-averaged LES/RANS results. The instantaneous snapshot also highlights the ability of the current model to resolve small scale fluctuations of vibrational temperature in the wake region. The extent of vibrational nonequilibrium is evident in the contours presented in Figure 5.13, where the difference between the translational/rotational temperature and the vibrational temperature are computed according to $T - T_v$. In this figure, regions colored in green represent, for the most part, regions where thermal equilibrium is established. Apart from the initial overshoot of translational/rotational temperature close to the bow-shock, the afterbody flow is mostly dominated by regions in which the vibrational temperature is greater than the translational/rotational temperature. Maximum temperature differences of approximately 2000 K, which is about 30% of the maximum post shock temperature $T$, are predicted by both models close to the leeside shoulder expansion. One capsule diameter from the base and further downstream, the vibrational temperature decreases towards equilibrium values, and is approximately 300-500 K higher than the translational/rotational temperature. The RANS results predict a recirculation region in which the translational/rotational temperature is greater (by approximately 300 K) than the vibrational temperature, whereas the time averaged LES/RANS contours show a recirculation region which is mostly in thermal equilibrium. The high fidelity model is able to resolve small scale turbulent structures, which results in enhanced mixing of the flow in the recirculation zone, and therefore the temperatures approach equilibrium much quicker in the LES/RANS results. At the particular instance shown though, the instantaneous contours show a similar degree of temperature differences in the recirculation zone.
Figure 5.12: Centerplane and out-of-plane slices showing vibrational temperature contours obtained from a) RANS, b) time-averaged LES/RANS, c) instantaneous LES/RANS.

Figure 5.13: Centerplane and out-of-plane slices showing extent of thermal nonequilibrium obtained from a) RANS, b) time-averaged LES/RANS, c) instantaneous LES/RANS.
The flowfield’s chemistry is also different depending on whether a RANS or an LES/RANS turbulence model is used. Figure 5.14 to Figure 5.17 show the mass fractions of $N_2$, $N$, NO, and O obtained using RANS and LES/RANS methods. Both turbulence models predict similar levels of $N_2$ dissociation in the forebody as expected, with only about 2% of the freestream $N_2$ being dissociated. In the afterbody wake though, the use of the LES/RANS model enhances the recombination of atomic species into molecular $N_2$, whereas RANS results show smaller $N_2$ mass fractions in the separated region. Additionally, RANS results show a larger amount of atomic $N$ in the recirculation region and along the separated shear layer than LES/RANS. Both models predict similar amounts of NO, peaking at mass fractions of $\sim 0.05$ near the shock, and leveling out at about 0.02 near the forebody. After the leeside expansion, some NO reaches the recirculation zone, where mass fractions similar to forebody values are seen. In general, the time-averaged LES/RANS results predict slightly larger NO levels in the wake. Finally, as expected, molecular oxygen gets dissociated almost entirely, resulting in large mass fraction values for atomic O in the post-shock flowfield. Mass fractions as high as 0.22 are found in the forebody region and are convected downstream as the flow expands. However, reduced O mass fractions are found in the recirculation region where recombination into molecular species is promoted. The high fidelity model is able to recombine greater amounts of molecular oxygen during the flow’s residence time inside the recirculation zone.

This study demonstrates the newly implemented ability of REACTMB to simulate high enthalpy flows in thermal nonequilibrium using an LES/RANS turbulence model. The results presented in this section highlight some of the differences in thermal and chemical nonequilibrium effects produced by a conventional RANS model as opposed to those obtained using a more physics-based, higher fidelity scheme.
Figure 5.15: Centerplane and out-of-plane slices showing atomic N mass fractions obtained from a) RANS, b) time-averaged LES/RANS, c) instantaneous LES/RANS.

Figure 5.16: Centerplane and out-of-plane slices showing NO mass fractions obtained from a) RANS, b) time-averaged LES/RANS, c) instantaneous LES/RANS.
Figure 5.17: Centerplane and out-of-plane slices showing atomic O mass fractions obtained from a) RANS, b) time-averaged LES/RANS, c) instantaneous LES/RANS.
Chapter 6

Summary and Conclusions

In this work, the performance of a hybrid LES/RANS turbulence model was evaluated for re-entry type blunt-body hypersonic wake flows. The initial literature survey showed that even though RANS models have been used for many years to simulate wake flows, they cannot accurately capture the physics of the separated afterbody region, which motivates the study of higher fidelity tools. It was also found that different turbulence models perform differently for different types of flows and different flow conditions, highlighting the need to validate this hybrid LES/RANS scheme for base flows. Given the rapid growth in computational power available to engineers, higher fidelity tools will eventually become practical design tools, and therefore current efforts to build confidence in these methods are of great importance. NC State’s hybrid LES/RANS model is assessed by using data from the CUBRC Mach 6 base flow experiments. Two different Reynolds numbers, one corresponding to a fully turbulent flow and a second corresponding to a nominally transitional flow, were simulated using a typical RANS model and the high fidelity LES/RANS model, with a calorically perfect air test gas. These test cases have been shown to be good candidates for validating turbulence models in the literature. In addition, the large range of turbulent scales present in the near wake, and the unsteady shear layer separating the recirculation region from the outer flow, make these types of flows very challenging cases for CFD codes. Pressure comparisons between the experiment and the simulations showed that all turbulence models, including RANS, are able to make good predictions within 1% of the stagnation pressure value. However, obtaining good agreement with heat transfer predictions proved to be much more difficult. No advantage was found to using high fidelity schemes such as LES/RANS and DES in attached flow regions, where RANS models provide results of similar accuracy. On the forebody, results for both Reynolds number cases showed an integrated error of approximately 30%. Along the attached windside afterbody, all models showed an average error of $\sim 50\%$ and $\sim 100\%$ for the fully turbulent and transitional cases, respectively. However, a great part of this error was due to the lack of a model for
transition. In the separated region, great improvements were shown by the LES/RANS model over the RANS approach. On the leeside backshell region, the integrated error was calculated to be \(~50\%\) and \(~60\%\) for the high and medium Reynolds number cases, respectively, using the LES/RANS. The corresponding average errors in this region obtained with the RANS model were much greater than twice that of LES/RANS for both cases.

Additionally, by comparing the results obtained for the fully turbulent test case using the LES/RANS PPM and the Low-Dissipation PPM schemes, it was found that both produced very similar results when comparing surface gauge data to the experiment. However, a qualitative look of the resulting flowfields showed that the low-dissipation scheme resolves turbulent structures in the wake which are closer in size to the resolution allowed by the grid, whereas the PPM scheme tends to dissipate a good deal of these structures. A new modification to the LES/RANS blending function was introduced to avoid erroneous transitioning behavior due insufficient grid resolution within boundary layers. This modification proved to be crucial in obtaining results which more closely matched the experiment, and to allow the model to respond as it was originally intended. Further studies into the scheme’s temporal accuracy showed that the LES/RANS model was able to reproduce some of the transients observed (trends and amplitudes) in the time-traces obtained from the experiment. However, additional grid refinement in the separated region could improve agreement. Finally comparisons with DES results provided by Dr. Barnhardt, demonstrated that the LES/RANS model can produce results which are as good as DES, and therefore providing an alternative approach to simulating complex base flows.

The second part of this work described the implementation and addition of thermal nonequilibrium capabilities to NC State’s REACTMB solver. A two-temperature vibrational nonequilibrium model, where one temperature governs the translational and rotational energy and the other governs the vibrational and electronic energy, was implemented. However, electronic energy was neglected in this work. Also, a 5-species air chemistry model was added where only 5 principal reactions are considered based on Park’s 1985 model. These additions required a good deal of modifications to the existing code structure, and therefore a verification study was conducted by performing code-to-code comparisons with NASA’s DPLR code. The results for a 2D half-cylinder confirmed the correct implementation of the thermal nonequilibrium and Park’s chemistry model in REACTMB, and excellent agreement was seen between REACTMB and DPLR. Finally, a more realistic three-dimensional simulation was performed of flow around a spherical capsule at a high Reynolds number condition to test the integration of the thermochemical nonequilibrium model with the existing LES/RANS turbulence model.

In the end, the work presented in this thesis evaluates a state-of-the-art turbulence model for simulating complex re-entry type flows, with the addition of thermochemical nonequilibrium capabilities. This high fidelity approach captures a good deal of the complex physical and
chemical interactions which occur during atmospheric re-entry. However, there is certainly room left for future improvements as modeling assumptions for turbulence, chemical-kinetics, and transition are revisited by the aerothermodynamics community in years to come.
References


Appendix
Appendix A

Species Data and Model Parameters

Table A.1: Species chemical data and characteristic vibrational temperature.

<table>
<thead>
<tr>
<th>Species</th>
<th>$M_n$(g/mol)</th>
<th>$h_n^o$(J/kg)</th>
<th>$\theta_{v,n}$(K)</th>
</tr>
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<tbody>
<tr>
<td>$N_2$</td>
<td>28.016</td>
<td>0.0</td>
<td>3395</td>
</tr>
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<td>$O_2$</td>
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<td>0.0</td>
<td>2239</td>
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<td>NO</td>
<td>30.008</td>
<td>$2.996213 \times 10^6$</td>
<td>2817</td>
</tr>
<tr>
<td>N</td>
<td>14.008</td>
<td>$3.362161 \times 10^7$</td>
<td>-</td>
</tr>
<tr>
<td>O</td>
<td>16.000</td>
<td>$1.543119 \times 10^7$</td>
<td>-</td>
</tr>
</tbody>
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Table A.2: Blottner curve fit coefficients for viscosity.

<table>
<thead>
<tr>
<th>Species</th>
<th>$A_n$</th>
<th>$B_n$</th>
<th>$C_n$</th>
</tr>
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<tbody>
<tr>
<td>$N_2$</td>
<td>0.0268142</td>
<td>0.317784</td>
<td>-11.3156</td>
</tr>
<tr>
<td>$O_2$</td>
<td>0.044929</td>
<td>-0.0826158</td>
<td>-9.20195</td>
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<td>NO</td>
<td>0.0436378</td>
<td>-0.0335511</td>
<td>-9.57674</td>
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<td>N</td>
<td>0.0115572</td>
<td>0.603168</td>
<td>-12.4327</td>
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<td>O</td>
<td>0.0203144</td>
<td>0.42944</td>
<td>-11.6031</td>
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Table A.3: Forward reaction rate coefficient parameters. (* * $C_{f,r}$ in units of mol,m,s,K.)

<table>
<thead>
<tr>
<th>Reaction(r)</th>
<th>$C_{f,r}$ * *</th>
<th>$\eta_r$</th>
<th>$\frac{E_{ar}}{R_u}$ (K)</th>
</tr>
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<tr>
<td>$N_2 + M \leftrightarrow N + N + M$</td>
<td>$3.70 \times 10^{18}$</td>
<td>-1.6</td>
<td>113200</td>
</tr>
<tr>
<td>$O_2 + M \leftrightarrow O + O + M$</td>
<td>$2.75 \times 10^{16}$</td>
<td>-1.0</td>
<td>59500</td>
</tr>
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<td>$2.30 \times 10^{14}$</td>
<td>-0.5</td>
<td>75500</td>
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<tr>
<td>$N_2 + O \leftrightarrow NO + N$</td>
<td>$3.18 \times 10^{10}$</td>
<td>0.1</td>
<td>37700</td>
</tr>
<tr>
<td>$NO + O \leftrightarrow O_2 + N$</td>
<td>$2.16 \times 10^5$</td>
<td>1.29</td>
<td>19220</td>
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Table A.4: Third body efficiency factors.

<table>
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<th>Reaction(r)</th>
<th>$TB_{N_2,r}$</th>
<th>$TB_{O_2,r}$</th>
<th>$TB_{NO,r}$</th>
<th>$TB_{N,r}$</th>
<th>$TB_{O,r}$</th>
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<tr>
<td>$N_2 + M \leftrightarrow N + N + M$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>3.0</td>
<td>3.0</td>
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<tr>
<td>$O_2 + M \leftrightarrow O + O + M$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>$NO + M \leftrightarrow N + O + M$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Table A.5: Equilibrium constant coefficients for Park 1985 model.

<table>
<thead>
<tr>
<th>Reaction(r)</th>
<th>$A_{1,r}$</th>
<th>$A_{2,r}$</th>
<th>$A_{3,r}$</th>
<th>$A_{4,r}$</th>
<th>$A_{5,r}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2 + M \leftrightarrow N + N + M$</td>
<td>3.898</td>
<td>-12.611</td>
<td>0.683</td>
<td>-0.118</td>
<td>0.006</td>
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<tr>
<td>$O_2 + M \leftrightarrow O + O + M$</td>
<td>1.335</td>
<td>-4.127</td>
<td>-0.616</td>
<td>0.093</td>
<td>-0.005</td>
</tr>
<tr>
<td>$NO + M \leftrightarrow N + O + M$</td>
<td>1.549</td>
<td>-7.784</td>
<td>0.228</td>
<td>-0.043</td>
<td>0.002</td>
</tr>
<tr>
<td>$N_2 + O \leftrightarrow NO + N$</td>
<td>2.349</td>
<td>-4.828</td>
<td>0.455</td>
<td>-0.075</td>
<td>0.004</td>
</tr>
<tr>
<td>$NO + O \leftrightarrow O_2 + N$</td>
<td>0.215</td>
<td>-3.652</td>
<td>0.843</td>
<td>-0.136</td>
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