ABSTRACT

POTTURI, AMARNATHA SARMA. Numerical Simulation of High-Speed Combustion Processes in Scramjet Configurations. (Under the direction of Dr. Jack R. Edwards.)

Flows through scramjet configurations are simulated using hybrid large-eddy simulation / Reynolds-averaged Navier-Stokes techniques. Present study is performed in three parts: parametric studies to determine the sensitivities of the predictions to modeling and algorithmic variations; formulation, implementation, and testing of several subgrid closures aimed at modeling filtered species production rates, which account for turbulence-chemistry interactions in a finite rate chemistry large-eddy simulation framework; and as a final assessment of the complete methodology, cavity-stabilized ethylene combustion is simulated. Throughout the present study, emphasis is placed on characterizing facility-specific effects, since they can have a significant influence on the numerical solution. In Part One, non-reactive and reactive flows through a model scramjet combustor with a wedge shaped injector are simulated. Different grids, flux reconstruction methods, reaction mechanisms, and inflow boundary conditions are used. To enhance fuel-air mixing, a synthetic eddy method is used to generate turbulence in the injector boundary layers and the hydrogen jets. The results show that in all the cases a lifted flame is predicted with varying standoff distances, heat releases, and shapes. In Part Two, the subgrid closures for modeling the filtered species production rates are tested on two different scramjet configurations with fundamentally different flow patterns and flame structures, one with the wedge shaped injector placed at the center of the combustor section (first, used in Part One), another with a three-dimensional ramp injector located on the upper wall of the combustor section (second). While the impact of these closures on the flow through the first configuration is insignificant, they have a more pronounced effect on the flow through the second configuration. Error analysis and performance quantification of these closures reveal that, relative to a baseline model, two of the closures improve the accuracy of the predictions, but the degree of improvement is quite modest. Also, from a cost-benefit perspective none of the models are a significant improvement over the ‘laminar-chemistry’ closure (where turbulence-chemistry interactions are ignored), for the configurations tested and the mesh resolutions employed. In Part Three, reactive flow through an ethylene fueled cavity flameholder is simulated using 14- and 22-species ethylene oxidation mechanisms, and the synthetic eddy method (used in Part Two) is used
to introduce turbulence at the inflow plane of the flameholder. For an equivalence ratio of 0.15, the 14-species mechanism resulted in a flame blow-out, and the 22-species mechanism predicted a cavity stabilized flame. Results predicted using the 22-species mechanism compare well with the experimental data, especially, water mole-fraction distribution and pressure along the upper wall of the combustor. In general, the predictions show excellent agreement with experimental data within the cavity region; further downstream, experimental results suggest that the heat release is over-predicted in the simulations.
Numerical Simulation of High-Speed Combustion Processes in Scramjet Configurations

by
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DEDICATION

To Kappagantula Venkata Subba Rao
and Vignesh Prakash
Amarnatha Sarma Potturi was born in 1987 in Hyderabad, Andhra Pradesh, India to Durga Prasada Rao Potturi and Venkata Lakshmi Potturi. After finishing grade school in Hyderabad, in 2004, he joined Indian Institute of Technology, Kharagpur in pursuit of a Bachelor of Technology degree in Aerospace Engineering. In 2008, he finished his undergraduate studies and joined the Master of Science in Aerospace Engineering program at North Carolina State University (NCSU). He defended his Master’s thesis in November of 2010, and continued his graduate studies at NCSU in pursuit of a Doctoral degree. During his time at NCSU, Amarnatha worked with Dr. Jack R. Edwards, first on simulations of electrosprays, and later on simulations of flows inside scramjet configurations. He plans to finish his Doctoral studies by the end of 2013.
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NOMENCLATURE

$(*)$  PaSR(1): fine-scale structures property

$(0)$  PaSR(1): coarse structures property

$(*)_i$  PaSR(1): property corresponding to the interface between fine-scale and coarse structures

$\beta$  Menter SST or BSL model constant

$\beta^*$  Menter SST or BSL model constant

$\acute{u}_j$  velocity fluctuation field

$\Delta s$  PaSR(1): diffusion length-scale

$\Delta$  average cell size

$\Delta_j$  cell size in the $j^{th}$ direction

$\delta_{ij}$  Kronecker delta

$\dot{\omega}_s$  production rate of species $s$

$\eta$  Arrhenius temperature exponent for $k_f$

$\Gamma$  blending function for LES/RANS

$\gamma$  Menter SST or BSL model constant

$\gamma^*$  PaSR(1): volume fraction of the fine-scale structures

$\kappa$  Menter SST or BSL model constant

$\kappa$  Von Kármán constant

$(\ )''$  density-weighted fluctuation

$(\ )'$  non-density-weighted fluctuation

$E^c$  convective component of the inviscid flux vector
\( \mathbf{E}^p \)  pressure component of the inviscid flux vector

\( \mathbf{F}_j \)  inviscid flux vector

\( \mathbf{G}_j \)  viscous flux vector

\( \mathbf{R}_s \)  steady residual

\( \mathbf{R}_u \)  unsteady residual

\( \mathbf{U} \)  vector of conservative variables

\( \mathbf{W} \)  vector of primitive variables

\( \mu \)  molecular viscosity

\( \mu_s \)  laminar viscosity of species \( s \)

\( \mu_t \)  eddy viscosity

\( \nu \)  kinematic viscosity

\( \nu''_{s,i} \)  stoichiometric coefficient of species \( s \)  in the \( i^{th} \) reaction on the products side

\( \nu'_{s,i} \)  stoichiometric coefficient of species \( s \)  in the \( i^{th} \) reaction on the reactants side

\( \Omega \)  vorticity magnitude or cell-volume

\( \omega \)  dissipation rate per unit turbulent kinetic energy

\( \Omega^* \)  \( \text{PaSR}(1) \): volume occupied by the fine-scale structures

\( \bar{\text{()}} \)  time-averaged or filtered quantity

\( \phi \)  blended set of model constants for the Menter SST or BSL models

\( \phi_1 \)  set of model constants for the \( k-\omega \) model

\( \phi_2 \)  set of model constants for the \( k-\epsilon \) model

\( \rho \)  total density of the mixture

\( \rho_s \)  density of species \( s \)
σ_k \quad \text{Menter SST or BSL model constant}

σ_ω \quad \text{Menter SST or BSL model constant}

σ_{ij} \quad \text{length scale of velocity component } u_i \text{ in the } j^{th} \text{ direction}

σ_{\text{max}} \quad \text{largest length scale}

τ_{ij} \quad \text{viscous stress tensor}

τ_{ij}^S \quad \text{subgrid stress tensor}

ε_{ij}^k \quad \text{intensity of the } j^{th} \text{ component of the } k^{th} \text{ eddy}

\bar{()} \quad \text{Favre-averaged or Favre-filtered quantity}

\bar{A} - \bar{G} \quad \text{flux Jacobians}

A^* \quad \text{PaSR(1): surface area of the fine-scale structures}

a_{ij} \quad \text{Cholesky decomposition of Reynolds stress tensor}

C \quad \text{Arrhenius pre-exponential for } k_f

C_M \quad \text{model constant for the subgrid eddy viscosity closure}

C_N \quad \text{model constant}

c_{1,2,3} \quad \text{model constants}

C_\mu \quad \text{model constant}

c_{p,s} \quad \text{specific heat per unit mass at constant pressure of species } s

D \quad \text{pipe diameter}

\epsilon_s \quad \text{internal energy per unit mass of species } s

E_{a,i} \quad \text{Arrhenius activation energy for } k_f

f \quad \text{scaling factor}

F_1 \quad \text{Menter SST or BSL blending function}
\( f_{\sigma_{ij}} \)  
shape function

\( G_i \)  
Gibbs free energy of the \( i^{th} \) reaction

\( G_j \)  
spatial filtering operator

\( g_s \)  
Gibbs free energy of species \( s \)

\( h \)  
enthalpy of the mixture per unit mass

\( h_s \)  
enthalpy per unit mass of species \( s \)

\( h_{f,s} \)  
enthalpy of formation per unit mass of species \( s \)

\( k_R \)  
resolved turbulent kinetic energy

\( k_{b,i} \)  
backward rate coefficient

\( k_{eq,i} \)  
equilibrium rate constant of the \( i^{th} \) reaction

\( k_{f,i} \)  
forward rate coefficient

\( l_i \)  
maximum boundary layer thickness along the \( i^{th} \) wall

\( M \)  
Mach number

\( N_A \)  
Avagadro constant

\( n_j \)  
\( j^{th} \) component of the normal vector

\( n_s \)  
number-density of species \( s \)

\( p \)  
pressure

\( Pr \)  
Prandtl number

\( q_c \)  
subgrid kinetic energy

\( q_j \)  
heat flux vector

\( q_{j_s} \)  
subgrid heat flux vector

\( r^+ \)  
non-dimensional radial wall distance
\[ R_i \] rate of the \( i^{th} \) reaction
\[ R^+_k \] forward reaction rate
\[ R^-_k \] backward reaction rate
\[ R_{ij} \] Reynolds stress tensor
\[ Re_\Delta \] subgrid scale Reynolds number
\( S \) strain rate
\( s_s \) entropy of species \( s \)
\( Sc \) Schmidt number
\( t \) time
\( t_m \) PaSR(1): diffusion time-scale
\( T_{\text{ref}} \) reference temperature
\( t_{\text{sgs}} \) mixing time-scale
\( u_j \) \( j^{th} \) velocity component
\( V_B \) volume of the bounding box
\( V_{s,j} \) \( j^{th} \) diffusion velocity component
\( V_{s,j}^S \) subgrid species diffusion velocity
\( x_j \) \( j^{th} \) spatial coordinate
\( X_s \) mole fraction of species \( s \)
\( y_d \) distance from the nearest wall
\( Y_s \) mass fraction of species \( s \)
\( \text{CD} \) column-density
\( \text{NS} \) total number of species
Chapter 1

Introduction

1.1 Motivation

Sustained hypersonic flight (Mach numbers higher than 6) through air-breathing propulsion systems has been a challenge motivating engineers over the past few decades. While rocket engines are the preferred choice for hypersonic flight right now, their need to carry oxidizer on-board significantly increases the overall weight of the vehicle, thereby decreasing the propulsion efficiency. An air-breathing propulsion system will help in circumventing this requirement by using the oxygen in the atmosphere as oxidizer.

Air-breathing engine designs, which operate efficiently at subsonic and supersonic speeds are turbojet engines and ramjets. Turbojet engines are comprised of a number of moving parts: a compressor, used to compress the incoming airstream; a combustion chamber, where fuel is injected, mixed with the incoming airstream, and the resultant mixture is expanded through combustion; a turbine, used to power the compressor; and a nozzle, where the combustion products are accelerated to provide propulsion. Unlike turbojet engines, ramjets do not use moving parts to compress the incoming air; they rely on the high speed of the incoming airstream to generate a shock-system, which is used to compress and decelerate the incoming airstream.

Due to this reliance, ramjets cannot operate efficiently (or cannot operate at all) at low Mach numbers. They perform most efficiently at Mach numbers around 3, and their efficiency decreases with further increase in the Mach number. Also, at Mach numbers greater than 6, trying to decelerate the incoming hypersonic airstream to subsonic speeds will result in extremely high amount of stresses (which exceed the structural limits of
the engine frame) and strong shock-waves (which are detrimental to overall combustion process inside the engine). To avoid this, after the initial compression and deceleration, the air-flow is allowed to be supersonic, leading to the design of supersonic combustion ramjets (scramjets). This means that fuel-air mixing and subsequent combustion must occur at supersonic speeds. Controlling this complex combustion process is one of the major challenges faced in the design of scramjet engines.

Since scramjets (like ramjets) rely on the shock-system developing at the inlet for compression and deceleration of the incoming air, they are not operable at low-speeds. This limitation means that for testing the performance of scramjet engines, they should first be accelerated to hypersonic speeds using other forms of propulsion. In the past, flight tests were performed using rocket engines provide this initial acceleration to hypersonic speeds. Future designs are looking at combined cycle propulsion systems, which make a transition from turbojet engines to ramjets to scramjets, depending on the vehicle speed. In either case, this need for other forms of propulsion systems means that flight tests are expensive and require complex coordination of transitions between different propulsion systems.

An alternative to flight tests are ground based experiments using high-speed wind tunnels. Because of the flow regimes in which the scramjet engines operate, it is extremely difficult and expensive to reproduce the flow conditions for substantial amounts of time and without any contamination in the flow field. Further difficulties in taking measurements without causing any intrusion to the flow make the choice of experimentally studying high-speed combustion processes even less attractive. Due to these technical challenges, it is currently not possible to assess the performance of a scramjet engine over its operational envelope using experimental methods alone.

Given these limitations to flight tests and experimental facilities, using Computational Fluid Dynamics (CFD) techniques as tools to aid in the design of hypersonic vehicles has become an attractive choice. While experiments are used to validate various physical models used in CFD, major design decisions are based on simulations. Over the past few decades, owing to the exponential increase in processor speed and memory capacity, CFD has become an affordable tool for studying complex flows, more so with the advent of parallel computing.

The computational methods used in CFD heavily rely on several models used to represent various physical processes. So it is essential that the quality and reliability of
these models be tested and that their shortcomings are well understood. The present study is an effort aimed at better understanding the performance and shortcomings of existing models for high-speed combustion, and an attempt to formulate and test various closures that model turbulence-chemistry interactions in a high Mach number, high turbulence-intensity environment.

1.2 RANS, LES, and DNS

In addition to fuel-air mixing and combustion occurring at supersonic speeds, complex processes such as shock-boundary layer, shock-flame, and shock-shock interactions characterize the combustion process in a scramjet. The cumulative effect of all these complex processes and finite-rate chemistry effects is that combustion inside a scramjet is a highly transient phenomenon.

In the past, Reynolds-averaged Navier-Stokes (RANS) techniques have been successfully used to design various hypersonic scramjet-powered vehicles such as NASA’s Hyper-X, the University of Queensland’s HyShot program, and the U.S. Air Force’s Scramjet Engine Demonstrator. A detailed account of the usage of RANS techniques in various scramjet programs is given in [10, 9]. However, the fact that the RANS techniques solve the time-averaged Navier-Stokes equations implies that they are best used to solve steady-state problems and are not necessarily able to handle the highly transient supersonic combustion processes occurring inside a scramjet.

In the turbulent combustion community, it is generally agreed upon that capturing the transience in scramjet flow-fields is necessary to improve the overall accuracy of CFD predictions. To this end, several techniques have been proposed, two of which are Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES). In DNS, all scales of turbulence relevant to the problem at hand are resolved using a fine enough mesh, which makes DNS more suitable for low Reynolds number flows. In LES, the large, energy containing, geometry dependent turbulent structures are directly captured, and the small-scale structures, which are universal, are filtered out and the effect they have on the overall flow is modeled. This distinction in the scales to be resolved and modeled is made based on the Reynolds number of the flow of interest. The resolution of the large scales of turbulence helps in capturing the transience in the flow to a certain extent. Due to the rapid increase in the computational power over the past decade, LES has become
more affordable, but the reliability and accuracy of LES remains to be firmly established for high-speed combustion problems.

In LES, several mathematical models and procedures are used to represent physical processes occurring in the flow-field and to increase the accuracy of the simulation. Among these models are reduced reaction mechanisms to model fuel oxidation, reconstruction schemes to increase the spatial accuracy of the discretization and to reduce numerical dissipation, and advanced closures for modeling the effects of unresolved (subgrid) fluctuations. There is a need for understanding the influences of these models and procedures on the overall ability of LES to predict the flow physics of interest.

1.3 Turbulent Combustion Modeling

While accepted closures exist for modeling molecular diffusion processes, viscous stresses, reaction rates, and subgrid-scale turbulent stresses, modeling of turbulence-chemistry interaction (especially for high-speed combustion processes) is an area of research that is not yet mature. Several models have been proposed and used to simulate flows involving turbulent combustion, four of which were used in simulations involving high-speed combustion with partial success:

1.3.1 Finite-Rate Chemistry Models

Combustion process is essentially comprised of several chemical reactions involving multiple reactants (or species). A straightforward approach to modeling combustion is to use a suitable reaction mechanism and to account for the mass-conservation of all the species involved in the reaction mechanism. Then, to account for turbulence-chemistry interactions, a closure can be used to model the filtered species production terms, which appear in each of the mass-conservation equations.

The practical issue with this approach is that the reaction mechanism can involve tens of species and hundreds of reactions, which is the case most of the times. This means solving tens of mass-conservation equations along with the three momentum-conservation and one energy-conservation equations. A reduced reaction mechanism, which represents the gist of the large number of chemical reactions relevant to a particular combustion problem, can be used to decrease the number of species that are to be dealt with.
Each species mass-conservation equation consists of a chemical source term, which accounts for the production or consumption of the species due to chemical reactions. In LES, this source term appears in its filtered form (LES), which should be modeled to account for the influences of subgrid fluctuations in species densities and temperature on the production rates. In most of works, which use a finite-rate chemistry framework with LES, these influences are either ignored (‘laminar-chemistry’ closure) or are modeled using a Partially Stirred Reactor (PaSR) type subgrid closure [11, 12], where a volume of reacting fluid is assumed to be comprised of reacting fine- and coarse-scale structures. These types of closures are described in more detail in §2.2.6. Another approach similar to the PaSR type closures is the Fractal Flame Modeling (FFM) approach [13], where it is assumed that reactions occur only in the fine-scale (Kolmogorov) structures.

Berglund et al. [14] used a PaSR type and the ‘laminar-chemistry’ subgrid closures in their simulations of supersonic combustion through a configuration studied at ONERA/JAXA; however, the influences of the subgrid closures used were inconclusive. Fureby et al. [15] utilized the same PaSR closure to simulate reacting flow through the Hyshot II scramjet combustor. The ‘laminar-chemistry’ subgrid closure was also used by Peterson et al. [16, 17] to simulate the SCHOLAR supersonic-combustion experiment [18]. They reported reasonable agreement with wall pressure distributions and experimental CARS images. Implicit Large-Eddy Simulation (ILES) techniques along with the ‘laminar-chemistry’ closure were applied to supersonic hydrogen flame of Cheng et al. [19] by Dauplain et al. [20] and Boivin et al. [21]. The FFM closure was used by Cecere et al. [22] to simulate the shock-boundary layer interactions in the HyShot II scramjet combustor. Edwards et al. [23] used the ‘laminar-chemistry’ closure and a ‘Gaussian quadrature’ closure in the simulations of the Burrows and Kurkov [24, 25] experiment of supersonic reacting wall jet. The ‘Gaussian quadrature’ closure is based on the finite-scale truncation-error analysis of Margolin and Shashkov [26], which relates a general filtered mean operator $\overline{f(\phi)}$ to the operator evaluated using filtered mean data $f(\overline{\phi})$. A comprehensive study of the reactive flows through various configurations of the University of Virginia’s scramjet combustion facility, which use hydrogen as the fuel, using ‘laminar-chemistry’ and other PaSR type subgrid closures, was performed by Fulton et al. [27, 28, 29, 9].
1.3.2 Flamelet Models

An alternate approach is to decouple the chemistry from the fluid flow, which is the basis for all flamelet-type models, where the flame is assumed to be a very thin layer (negligible compared to the length scales of the flow) between fuel and oxidizer. This assumption makes it convenient to separate turbulent mixing from combustion chemistry. In flamelet modeling, details of multi-component diffusion-reaction processes are mapped to a small number of tracking scalars. So by solving the advection-diffusion equations for these tracking scalars, complete chemical state information can be obtained using the mapping procedure developed.

As described in Larsson et al. [30], the main issue with using flamelet modeling for supersonic combustion is that the dependence of chemical source terms on the variations in pressure and enthalpy is not accounted for. The fact that the flamelet library, which used to map the tracking scalars to the species mass-fractions and temperature, is precomputed (by assuming a reference pressure and temperatures at the fuel and oxidizer boundaries) means that there is no feedback from the LES solver to the flamelet library. This lack of feedback can lead to inaccuracies, especially when applied to supersonic combustion.

One of the most popular approaches successfully used in simulation of supersonic combustion is the Progress-Variable Approach (PVA) due to Pierce and Moin [31]. In this approach, transport equations are solved for three tracking scalars: the filtered mixture fraction, the subfilter variance of the mixture fraction, and reaction progress-variable. This approach was used by Larsson et al. [30] and Larsson [32] for simulating high-speed combustion in the Hyshot II scramjet combustor. Following the approach of Pecnik et al. [33], they assumed that the species mass-fractions are independent of the variations in pressure and temperature at the flamelet boundaries, instead, to account for these variations in some sense, they assumed that the source term of the reaction progress-variable scales with the square of pressure. They modeled the effect of subgrid-scale turbulence on the chemistry using a presumed $\beta$ Probability Density Function (PDF) for the mixture fraction. They acknowledge the inability of this approach to predict auto-ignition and the lack of feedback (of pressure and enthalpy variations) from the LES solution to the flamelet library; however, the predicted pressure-rise is within the experimental bounds.

Berglund et al. [34] used a one-equation flamelet model (without the advection-diffusion equations for the reaction progress-variable and its variance) for LES of reactive flow
through the DLR scramjet combustor [35, 36, 8]. They reported reasonable qualitative predictions with some discrepancies (compared to experimental results) in the degree of volumetric expansion of the flame and time-averaged velocity profiles.

1.3.3 Linear Eddy Model (LEM)

The linear eddy model was originally proposed by Kerstein [37, 38, 39], which was later developed into subgrid models for mixing and combustion by Menon et al. [40, 41] and Chakravarthy & Menon [42]. The model explicitly distinguishes between the effects of turbulent stirring, molecular diffusion, and chemical reactions at all length scales. The influences of molecular diffusion and chemical reactions to subgrid-scale transport are resolved using a one-dimensional domain, which is aligned along the direction of maximum scalar gradient. These models are generally computationally more expensive compared to finite-rate chemistry and flamelet-type models. Also, molecular diffusion across cell interfaces is ignored and various other simplifying assumption are made. In spite of these simplifying assumptions, LEM models were successfully used in the simulations of flows involving turbulent mixing [43, 44], non-premixed combustion [45, 46], and premixed combustion [47, 48].

1.3.4 Probability Density Function Approach

The Probability Density Function (PDF) [49] approach to turbulent combustion is based on solving a modeled transport equation for one-point, one-time Eulerian joint PDF of a set of variables that describe the thermochemical state of a reacting fluid [50]. By doing this, the species production rates appear in closed form and do not require any modeling. PDF methods were used in RANS simulations of supersonic turbulent combustion by Baurle et al. [51, 52, 53, 54] and Gerlinger [55]. In LES, the PDF approach is termed as Filtered-Density Function (FDF); while PDFs have been used in simulations of flows involving subsonic combustion, to the best of the author’s knowledge, they have not yet been applied to supersonic combustion problems.

A detailed description of the modeling philosophies described above and their application to LES of supersonic-combustion can be found in [56, 57].
1.4 Chemistry Modeling

Since finite-rate chemistry effects play an important role in supersonic combustion (due to comparable residence and chemistry time-scales), choosing an appropriate reaction mechanism to represent the combustion process is crucial. In a finite-rate chemistry framework, the fact that a large number of species can be involved in a combustion process means numerically solving a large number of transport equations. To overcome this, several reduced reaction mechanisms, which involve a limited number of species, have been proposed.

For supersonic hydrogen combustion, the most commonly used reduced reaction mechanisms are two nine-species, nineteen step mechanisms [58, 2] due to Jachimowski and a nine-species twenty one-step reaction mechanism due to ´O Connaire et al. [5]. While the Jachimowski reaction mechanism was successfully used in many works involving supersonic combustion of hydrogen, the mechanism due to ´O Connaire et al. is considered as being more comprehensive. A more recent trend in the development of hydrogen oxidation mechanisms is the inclusion of pathways that accurately predict combustion characteristics at high pressures (2 to 10 atm). An example is the mechanism of Burke et al. [6], which is used in one of the cases considered in the present study.

Gerlinger et al. [1] performed a validation experiment for supersonic hydrogen combustion with respect to various reduced reaction mechanisms (listed in Table 1.1). They found that for temperatures less than 1052 K and at a pressure of approximately 1 bar, detailed mechanisms (all the nine-species mechanisms) outperform the one- [59] and seven-species [60] mechanisms; and the ignition delay times predicted by the detailed mechanisms differed by nearly one order of magnitude. The one-step mechanism, even at less critical conditions (temperatures greater than 1052 K and at a pressure of 1 bar), was found to predict wrong ignition delay times, whereas the seven-species mechanism performed decently at these conditions. The Vajda et al. [61] mechanism was found to be too fast compared to experiments, and the GRI3.0 mechanism too slow. Overall, the ´O Connaire et al. [5] and the Jachimowski [2] mechanisms outperformed all other mechanisms. They also found that the presence of radicals in the freestream makes a significant difference in the predictions; so, for experiments using vitiated heaters to raise the air-stream temperature, consideration of freestream radicals in the simulations is recommended.

With so much variation in the predicted ignition delay times with respect to the reduced reaction mechanisms used, it is vital that an appropriate and computationally
Table 1.1: Hydrogen-air reaction mechanisms tested in Gerlinger et al. [1]

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Species</th>
<th>Steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jachimowski-1 [58]</td>
<td>9</td>
<td>19</td>
</tr>
<tr>
<td>Jachimowski-2 [60]</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Jachimowski [2]</td>
<td>9</td>
<td>19</td>
</tr>
<tr>
<td>Vajda et al. [61]</td>
<td>9</td>
<td>19</td>
</tr>
<tr>
<td>Ó Connaire et al. [5]</td>
<td>9</td>
<td>21</td>
</tr>
<tr>
<td>GRI3.0 [62]</td>
<td>9</td>
<td>29</td>
</tr>
<tr>
<td>Marinov et al. [59]</td>
<td>4</td>
<td>1</td>
</tr>
</tbody>
</table>

effective reaction mechanism is used in supersonic combustion. In the present work, the Jachimowski reaction mechanism [2], a seven-species seven-step abridged Jachimowski mechanism [4, 3], the Ó Connaire et al. reaction mechanism [5], and the reaction mechanism of Burke et al. [6] are used to model hydrogen oxidation.

The current state of the reduced reaction mechanisms accounting for ethylene-air kinetics is not as mature as it is for hydrogen-air kinetics. In the present study, two of the more comprehensive reduced ethylene oxidation mechanisms, a modified version of the 14-species 40-step mechanism of Gokulakrishnan et al. [7] and a 22-species mechanism [63, 64], are used. Details of all the mechanisms used in the present study (except for the 22-species ethylene oxidation mechanism) are listed in Appendix A.
1.5 Scope of the Present Study

The present study can be divided into three parts:

- The first part is a systematic investigation of the effects of various modeling and algorithmic modifications on the predictive capability of the LES/RANS solver REACTMB, developed at the North Carolina State University’s (NCSU) Aerospace Engineering CFD lab, as applied to the flow in a model scramjet combustor.

- The second part concerns the development and testing of several closures for the effects of un-resolved turbulent fluctuations on species production rates. These closures were tested on two different scramjet configurations.

- The third part involves the application of the REACTMB solver to simulate cavity-stabilized ethylene-air combustion.

In all cases, predictions are compared with available experimental data. Underpinning all these efforts is the development of an enhanced version of REACTMB that contains:

1. A platform independent implementation of a modified synthetic turbulence generation method based on the synthetic eddy method of Jarrin et al. [65].

2. Modules that incorporate various subgrid-scale closures for filtered species production rates.

3. Reduced ethylene-air reaction mechanisms.

4. Real-time visualization capability using Lawrence Livermore National Laboratory’s (LLNL) VisIt visualization tool (https://wci.llnl.gov/codes/visit/) \(^1\).

The current dissertation is organized as follows. In Chapter 2, the working set of equations and various models used to close the set of equations are presented. In Chapter 3, the numerical methods used to discretize and solve the system of equations are discussed. Chapter 4 describes the three scramjet experiments considered in the present study. Results from the three parts of the present study are presented in Chapters 5, 6, and 7, respectively. Finally, in Chapter 8, the work done in the present study is summarized and concluding remarks are presented.

\(^1\)Details regarding the integration of VisIt into REACTMB are given in Appendix C.
Chapter 2

Governing Equations

2.1 Multi-Species Navier-Stokes Equations for Reacting Gaseous Mixtures

Flow inside a scramjet is characterized by chemically reacting gaseous mixtures and is governed by the Navier-Stokes equations. In the current framework, it is assumed that each species in the gaseous mixture is a thermally perfect gas and that the mixture is in thermal equilibrium. Also, the influence of external body forces on the flow is neglected. The Navier-Stokes equations for a mixture of NS reacting gaseous species can be written as:

**Mass conservation of species** $s$:

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho_s (u_j + V_{s,j}) \right] = \dot{\omega}_s$$  (2.1)

where $s$ varies from 1 to NS. The above equation essentially means that the rate of change of mass of species $s$, at a point in space, is due to the bulk flow (represented by the fluid velocity $u_j$), diffusion processes (represented by the diffusion velocity $V_{s,j}$ of species $s$), and chemical reactions (represented by the species production rate due to chemical reactions $\dot{\omega}_s$).

**Momentum conservation**:

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho u_i (u_j + V_{s,j}) \right] = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$  (2.2)
Simply put, the momentum conservation equation means that change in the \(i^{th}\) component of momentum is due to the fluid flow (\(u_i\)), work done by the pressure (\(p\)), and work done by viscous stresses (\(\tau_{ij}\)).

**Energy conservation:**

\[
\frac{\partial}{\partial t} \left[ \sum_s \rho_s e_s + \frac{1}{2} \rho u_i u_i \right] + \frac{\partial}{\partial x_j} \left[ u_j \left( \sum_s \rho_s h_s + \frac{1}{2} \rho u_i u_i \right) \right] = -\frac{\partial q_j}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \sum_s \rho_s h_s V_{s,j} \right] \tag{2.3}
\]

The above set of equations essentially consists of: NS mass, three momentum (one in each coordinate direction), and one energy conservation equations. To close this set of (NS+4) equations, additional closures are required for defining internal energy per unit mass of species \(s\) (\(e_s\)), enthalpy per unit mass of species \(s\) (\(h_s\)), viscous stress tensor (\(\tau_{ij}\)), diffusion velocity of species \(s\) (\(V_{s,j}\)), pressure (\(p\)), and production rate of species \(s\) due to chemical reactions (\(\dot{\omega}_s\)), which are described below.

### 2.1.1 Assumptions and Closures

Given that all NS gaseous species occupy the same volume, the total density of the mixture (\(\rho\)) can be written as the sum of individual species densities (\(\rho_s\)):

\[
\rho = \sum_s \rho_s \tag{2.4}
\]

The internal energy per unit mass of species \(s\) is given by

\[
e_s = h_s - \frac{p_s}{\rho_s} \tag{2.5}
\]

where \(h_s\) is the enthalpy per unit mass of species \(s\).
Dalton’s Law of Partial Pressures

Following Dalton’s law of partial pressures, total pressure \( p \) of the gaseous mixture is expressed as the sum of partial pressures \( p_s \) of individual species:

\[
p = \sum_s p_s
\]

(2.6)

Partial pressures of individual species are then calculated using the ideal gas law:

\[
p_s = \rho_s R_s T \quad \text{and} \quad R_s = \frac{R_u}{W_s}
\]

(2.7)

where \( R_u \) is the universal gas constant, \( W_s \) is the molecular weight of species \( s \), and \( R_s \) is the specific gas constant for species \( s \).

Species Diffusion

Fick’s law is used to account for species diffusion while assuming a constant Schmidt number \( (Sc) \) of 0.5:

\[
V_{s,j} = \frac{1}{\rho_s} \frac{\mu}{Sc} \frac{\partial Y_s}{\partial x_j}
\]

(2.8)

where \( \mu \) is the molecular viscosity of the mixture of gases and \( Y_s \) is the mass fraction of species \( s \), which is defined as

\[
Y_s = \frac{\rho_s}{\rho}
\]

(2.9)

Thermally Perfect Gas Assumption

Total enthalpy of the mixture is given by

\[
h = \sum_s Y_s h_s
\]

(2.10)

where enthalpy per unit mass of species \( s \) is defined as

\[
h_s = h_{f,s} + \int_{T_{ref}}^T c_{p,s} dT
\]

(2.11)

In the above equation, \( h_{f,s} \) is the enthalpy of formation per unit mass of species \( s \)
and \( c_{p,s} \) is the specific heat of species \( s \). To define the species specific heat, each gaseous species is assumed to be thermally perfect, which means that species specific heat is a function of temperature alone. The specific form of this function used in the present study is obtained from the McBride et al. [66] curve fits:

\[
c_{p,s} = R_s \left[ A_s + B_s T + C_s T^2 + D_s T^3 + E_s T^4 \right]
\]

(2.12)

where the constants \( A_s \) through \( E_s \) are the curve fit coefficients for species \( s \).

**Mixture Molecular Viscosity**

Wilke’s law is used to calculate the mixture molecular viscosity:

\[
\mu = \frac{\sum_i X_i \mu_i}{\sum_j X_j \phi_{ij}} \quad \text{and} \quad \phi_{ij} = \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \left( \frac{W_i}{W_j} \right)^{\frac{1}{4}} \right]^2 \sqrt{8 \left( 1 + \frac{W_i}{W_j} \right)}
\]

(2.13)

where \( X_i \) is the mole fraction of species \( i \):

\[
X_s = \frac{\rho_s}{\sum_i \rho_i}
\]

(2.14)

In Equation 2.13, \( \mu_i \) is the laminar viscosity of species \( i \) and is calculated using Sutherland’s law:

\[
\mu_i = \mu_{ref,i} \left( \frac{T}{T_{\mu_i}} \right)^{\frac{3}{2}} \frac{T_{\mu_i} + S_{\mu_i}}{T + S_{\mu_i}}
\]

(2.15)

Values of \( \mu_{ref,i} \), \( T_{\mu_i} \), and \( S_{\mu_i} \) for individual species relevant to the present work are listed in Appendix B.

**Heat Conduction**

The heat transfer flux is calculated using the Fourier’s law of heat conduction extended for multiple species:

\[
q_j = -\frac{\mu}{Pr} \left( \sum_s Y_{s,c_{p,s}} \right) \frac{\partial T}{\partial x_j}
\]

(2.16)

where \( Pr \) is the Prandtl number, which is set to 0.72 in the present work.
Viscous Stresses

It is assumed that the mixture of gases is a Newtonian fluid and Stokes’ hypothesis is used to evaluate the viscous stress tensor:

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \tag{2.17}
\]

where \( \delta_{ij} \) is the Kronecker delta.

Species Production Rates

Assuming that the \( i^{th} \) chemical reaction can be written in the generic form shown below,

\[
\sum_s \nu'_{s,i} N_s \leftrightarrow \sum_s \nu''_{s,i} N_s \tag{2.18}
\]

The rate of production of species \( s \) can be written as:

\[
\dot{\omega}_s (\rho_s, T) = W_s \sum_i \left( \nu''_{s,i} - \nu'_{s,i} \right) R_i \tag{2.19}
\]

where \( R_i \) is the rate of the \( i^{th} \) reaction, which is calculated using the law of mass action:

\[
R_i = k_{f,i} \prod_i \left( \frac{\rho_s}{W_s} \right)^{\nu'_{s,i}} - k_{b,i} \prod_i \left( \frac{\rho_s}{W_s} \right)^{\nu''_{s,i}} \tag{2.20}
\]

In the above equation, \( k_{f,i} \) and \( k_{b,i} \) are the forward and backward rate coefficients of the \( i^{th} \) reaction, respectively, and \( k_{f,i} \) is calculated using the Arrhenius equation:

\[
k_{f,i} = C_i (T)^{\eta_i} \exp \left[ -\frac{E_{a,i}}{R_u T} \right] \tag{2.21}
\]

where \( C_i, \eta_i, \) and \( E_{a,i} \) are the Arrhenius pre-exponential coefficient, Arrhenius temperature exponent, and Arrhenius activation energy for the \( i^{th} \) reaction, respectively. Backward rate coefficient of the \( i^{th} \) reaction is related to \( k_{f,i} \) using the equilibrium rate constant \( (k_{eq,i}) \):

\[
k_{b,i} = \frac{k_{f,i}}{k_{eq,i}} \tag{2.22}
\]
The change in the Gibbs free energy ($\Delta G_i$) for the $i^{th}$ reaction is used to calculate $k_{eq,i}$:

$$k_{eq,i} = \left(101325 \frac{R_u}{T}\right)^{\frac{m'' - m'}{m''}} \exp \left(\frac{\Delta G_i}{R_u T}\right)$$ (2.23)

where

$$\Delta G_i = \sum_s \left(\nu''_{s,i} - \nu'_{s,i}\right) g_s$$ (2.24)

$$g_s = h_s - T s_s$$ (2.25)

$$m' = \sum_s \nu'_{s,i} \quad \text{and} \quad m'' = \sum_s \nu''_{s,i}$$ (2.26)

Entropy ($s_s$) of species $s$ is calculated using the McBride et al. [66] curve fits:

$$s_s = R_u \left[ A_s \ln T + B_s T + C_s \frac{T^2}{2} + D_s \frac{T^3}{3} + E_s \frac{T^4}{4} + G_s \right]$$ (2.27)

where the constants $A_s$ through $G_s$ are the curve fit coefficients for species $s$.

**Third-Body Reactions:** Also, third-body reactions are routinely part of many reaction mechanisms, where essentially a third body aids in the dissociation of a molecule or in the recombination of a set of molecules. The generic form of a third body reaction is shown below:

$$AB + M \leftrightarrow A + B + M$$ (2.28)

Here $M$ can be any one of the NS species. So, the above reaction essentially represents NS third-body reactions. Instead of dealing with NS independent reactions, the rate of production of species $s$ due to NS third-body reactions can be expressed as:

$$\dot{\omega}_s(\rho_s, T) = W_s \left(\nu'' - \nu'\right) \left[ \left(\sum_i k_{f,i} \frac{\rho_i}{W_i}\right) \frac{\rho_{AB}}{W_{AB}} - \left(\sum_i k_{b,i} \frac{\rho_i}{W_i}\right) \frac{\rho_A \rho_B}{W_A W_B} \right]$$ (2.29)

where $i$ varies from 1 to NS. For a third-body reaction, the forward and backward rate coefficients ($k_{f,i}$ and $k_{b,i}$) can be expressed as products of the rate coefficients of the original dissociation/recombination reaction ($k_f$ and $k_b$) and Chaperon efficiencies of species $i$, (TB)$_i$:

$$k_{f,i} = k_f(TB)_i \quad \text{and} \quad k_{b,i} = k_b(TB)_i$$ (2.30)
Substituting the above two terms in Equation 2.29, the production rate of species \( s \) due to NS third-body reactions can be written as:

\[
\dot{\omega}_s (\rho_s, T) = W_s \left( \nu_s'' - \nu_s' \right) \left[ k_f \frac{\rho_{AB}}{W_{AB}} - k_b \frac{\rho_A}{W_A} \frac{\rho_B}{W_B} \right] \sum_i (TB)_i \frac{\rho_i}{W_i} \tag{2.31}
\]

**Pressure Dependence:** Based on the above formulation, it can be said that the reaction rates are functions of temperature alone. However, the rates of certain reactions strongly depend on pressure variations. This pressure dependence is accounted for by blending the forward rate coefficients at high and low pressures \( k_{f,\infty} \) and \( k_{f,0} \), respectively to calculate the overall forward rate coefficient:

\[
k_f = k_{f,\infty} \left( \frac{p_r}{1 + p_r} \right) F \tag{2.32}
\]

where \( k_f \) is the overall forward rate coefficient and \( p_r \) is the reduced pressure, which is defined as:

\[
p_r = \frac{k_{f,0} C_{mix}}{k_{f,\infty}} \tag{2.33}
\]

where

\[
C_{mix} = \frac{\rho_{mix}}{W_{mix}} \tag{2.34}
\]

\[
W_{mix} = \sum_s X_s W_s \quad \text{and} \quad \rho_{mix} = \sum_s \rho_s \tag{2.35}
\]

Function \( F \) in Equation 2.32 is defined as:

\[
\ln(F) = \left\{ 1 + \left[ \frac{\ln(p_r) + c}{n - d(\ln(p_r) + c)} \right]^2 \right\}^{-1} \ln(F_{cent}) \tag{2.36}
\]

where

\[
c = -0.4 - 0.67 \ln(F_{cent}), \quad n = 0.75 - 1.27 \ln(F_{cent}), \quad \text{and} \quad d = 0.14 \tag{2.37}
\]

\[
F_{cent} = (1 - a) \exp \left( \frac{-T}{T_{**}} \right) + a \exp \left( \frac{T}{T^*} \right) + \exp \left( \frac{-T_{**}}{T} \right) \tag{2.38}
\]

In the present study, four different reaction mechanisms (Jachimowski [2], a seven-species reaction mechanism [3, 4], Ó Connaire et al. [5], and Burke et al. [6]) are used for hydrogen combustion. For ethylene-air kinetics, two different reduced mechanisms (Gokulakrishnan et al. [7] and the Taitech-Princeton 22-species mechanism [63, 64]) are used. Detailed
steps involved in each of these mechanisms (except for the Taitech-Princeton mechanism) and values of various Arrhenius constants \((C, \eta, \text{ and } E_a)\), third-body coefficients \((\text{TB})\), and constants required to evaluate the pressure dependence of certain steps \((a, T^*, T^{**}, \text{ and } T^{***})\) are all listed in Appendix A.

## 2.2 Turbulence Modeling

The Navier-Stokes equations presented in the previous section, along with the closures for various terms appearing in the equations, can be solved directly using a mesh fine enough to resolve all scales of turbulence. The number of mesh cells required over a volume of \(L^3\) scales with respect to the Reynolds number as \(\text{Re}^{9/4}\). For flows with high Reynolds numbers, this requirement in the mesh resolution results in very high cell counts, which are impractical to deal with. This is the case with most flows of practical interest, and to avoid dealing with such high cell counts, in the present work, two different approaches are used: RANS and LES/RANS, which are described below.

### 2.2.1 Reynolds-Averaged Navier-Stokes (RANS) Equations

Reynolds-averaged Navier-Stokes equations are derived by time-averaging the Navier-Stokes equations. The idea is to eliminate the temporal fluctuations in the quantities by time-averaging the equations. While the temporal fluctuations are eliminated, the influences of these fluctuations on the mean flow appear in the form of additional terms. The derivation of the RANS equations and the closures for the additional terms are described in this section.

The time-average \(\overline{q}(x_i)\) of a generic quantity \(q(x_i, t)\) is calculated as shown below:

\[
\overline{q}(x_i) = \frac{1}{\Delta t} \int_t^{t+\Delta t} q(x_i, t')dt'
\]  

Using the above notation, the generic quantity can then be expressed as a sum of the time-averaged quantity \(\overline{q}\) and a fluctuation part \(q'\):

\[
q = \overline{q} + q'
\]
For compressible flows, the time-averaging operation will result in a number of correlations between $\rho'$ and other flow quantities. To close the system, closures should be formulated for all these correlations. To cut down on the number of correlations for which closures are required, a density based averaging technique is used, which is shown below:

$$\tilde{q} = \frac{\overline{pq}}{\overline{p}}$$ (2.41)

The generic quantity $q$ can then be expressed as a sum of the density based time-averaged quantity ($\tilde{q}$) and a density based fluctuation quantity ($q''$):

$$q = \tilde{q} + q'' \quad \text{and} \quad \tilde{q}'' = 0$$ (2.42)

This kind of density based averaging is called Favre-averaging, and the Favre-averaged Navier-Stokes equations are shown below:

**Mass conservation:**

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_j} \left[ \overline{\rho} \left( \tilde{u}_j + \tilde{V}_{s,j} \right) + \overline{\rho '' Y''_{s,j}} + \overline{\rho '' Y''_{s,j}} \right] = 0$$ (2.43)

**Momentum conservation:**

$$\frac{\partial (\overline{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} \left[ \overline{\rho \tilde{u}_j \tilde{u}_i} \right] = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \tau_{ij} \right]$$ (2.44)

**Energy conservation:**

$$\frac{\partial}{\partial t} \left[ \sum_s \left( \overline{p_s} \tilde{h}_s + \overline{\rho'' Y'' s} \right) + \frac{1}{2} \overline{\rho \tilde{u}_i \tilde{u}_i} + \frac{1}{2} \overline{\rho'' u''_i u''_i} \right]$$

$$+ \frac{\partial}{\partial x_j} \left[ \tilde{u}_j \sum_s \left( \overline{p_s \tilde{h}_s} \right) + \sum_s \left( \tilde{Y''_{s, i} \rho''_{s, i} u''_{s, i} + \tilde{h}_{s, i} \rho''_{s, i} Y''_{s, i} + \tilde{h}_{s, i} \rho''_{s, i} Y''_{s, i} \right) \right]$$

$$+ \frac{\partial}{\partial x_j} \left[ \frac{1}{2} \tilde{u}_j \overline{\rho \tilde{u}_i \tilde{u}_i} + \overline{\rho'' u''_i \tilde{u}_i} + \frac{1}{2} \overline{\rho'' u''_i \tilde{u}_i} \right] = -\frac{\partial \tilde{q}_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \tau_{ij} + \tilde{u}_i \tau_{ij} \right]$$

$$- \frac{\partial}{\partial x_j} \left[ \sum_s \left( \overline{p_s \tilde{h}_s \tilde{V}_{s,j}} \right) + \sum_s \left( \tilde{Y''_{s,j} \rho''_{s,j} Y''_{s,j} + \tilde{h}_{s,j} \rho''_{s,j} Y''_{s,j} + \tilde{h}_{s,j} \rho''_{s,j} Y''_{s,j} \right) \right]$$ (2.45)

The additional correlations appearing in the Favre-averaged Navier-Stokes equations are
highlighted in green. Some of these terms are neglected and others are modeled using various hypotheses, which are described below:

**The Reynolds stress tensor** represents an increase in the overall viscosity of the fluid due to turbulence, which is modeled as shown below:

\[-\rho u_i''u_j'' \equiv \tau_{ij}^t = \mu_t \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu_t \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} - \frac{2}{3} \rho k \delta_{ij}^{0}\]  

(2.46)

where \(\mu_t\) is the turbulent eddy viscosity, which is representative of the additional viscosity due to turbulence, and is modeled using the turbulence models described in §2.2.2.

**Species diffusion due to turbulence:**

\[\rho Y_s''u_j'' \equiv p_s V_{s,j}^t = -\mu_t \frac{\partial \tilde{Y}_s}{\partial x_j}\]  

(2.47)

where \(Sc_t\) is the turbulent Schmidt number, which is set to 0.5 in the present work.

**The mass-specific turbulent kinetic energy**, shown below, appears in the Favre-averaged Navier-Stokes equations and is modeled using the turbulence closures described in §2.2.2:

\[\frac{1}{2} \rho u_i''u_i'' \equiv \bar{p}k\]  

(2.48)

**Turbulent heat flux (modeled):**

\[\sum_s \tilde{h}_s \rho u_j''Y_s'' \equiv q_j^t = -\mu_t \left( \sum_s \tilde{Y}_s \tilde{c}_{p,s} \right) \frac{\partial \tilde{T}}{\partial x_j}\]  

(2.49)

where \(Pr_t\) is the turbulent Prandtl number, which is set to 0.9 in the present work.

**Energy transport due to turbulent diffusion (modeled):**

\[\sum_s \tilde{h}_s \rho u_j''Y_s'' \equiv \sum_s \bar{p}_s \tilde{h}_s V_{s,j}^t\]  

(2.50)

where \(V_{s,j}^t\) is calculated using Equation 2.47.

**Molecular diffusion (neglected):**

\[\overline{u_i'' \tau_{ij}}\]  

(2.51)
Turbulent transport of turbulent kinetic energy (neglected):

\[
\frac{1}{2} \rho u_i u_i' u_i'
\] (2.52)

Replacing the above terms with their equivalent terms:

\[
\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho_s \left( \tilde{u}_j + \tilde{V}_{s,j} \right) + \rho_s V_{s,j}^t \right] = \bar{\omega}_s
\] (2.53)

\[
\frac{\partial (\bar{p} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} [\bar{p} \tilde{u}_j \tilde{u}_i] = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} [\tau_{ij} - \tau_{ij}]
\] (2.54)

\[
\frac{\partial}{\partial t} \left[ \sum_s \bar{p}_s \tilde{e}_s + \frac{1}{2} \bar{p} \tilde{u}_i \tilde{u}_i + \bar{p} \right] + \frac{\partial}{\partial x_j} \left[ \tilde{u}_j \left( \sum_s \bar{p}_s \tilde{h}_s + \frac{1}{2} \bar{p} \tilde{u}_i \tilde{u}_i + \bar{p} \right) \right]
= -\frac{\partial}{\partial x_j} \left[ \tilde{a}_j + d_j^t \right] + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \left( \tau_{ij} + \tau_{ij} \right) \right] - \frac{\partial}{\partial x_j} \left[ \sum_s \bar{p}_s \tilde{h}_s \left( \tilde{V}_{s,j} + V_{s,j}^t \right) \right]
\] (2.55)

### 2.2.2 RANS Turbulence Closure

To close the RANS equations described above, turbulent kinetic energy \((k)\) and turbulent eddy viscosity \((\mu_t)\) need to be calculated. To this end, the Menter BSL (baseline) model [67], which is a two-equation turbulence model, is used. The Menter BSL model is essentially a blend of the \(k - \omega\) and \(k - \epsilon\) models. The blending is done in such a way that the \(k - \omega\) model is used in the sublayer and the logarithmic regions of the boundary layer, and the \(k - \epsilon\) model is used in the wake region. This is done because of the superior performance of the \(k - \omega\) model in the sublayer and logarithmic regions of the boundary layer. In the wake region, the \(k - \omega\) model is highly sensitive to the freestream values of \(\omega\), and the \(k - \epsilon\) model does not suffer from this deficiency. As a result, in the wake region, the \(k - \epsilon\) model is the preferred choice. The \(k - \epsilon\) model is rewritten in terms of \(k\) and \(\omega\), and then the two models are blended together.

**Menter BSL Model**

\[
\frac{\partial \bar{p} k}{\partial t} + \tilde{u}_j \frac{\partial \bar{p} k}{\partial x_j} = \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} - \beta^* \bar{p} \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right]
\] (2.56)
\[
\frac{\partial \bar{\omega}}{\partial t} + \bar{u}_j \frac{\partial \bar{\omega}}{\partial x_j} = \frac{\gamma}{\nu_t} \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \beta \bar{\omega}^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] \\
+ 2 (1 - F_1) \bar{\rho} \sigma_{\omega 2} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \tag{2.57}
\]

where \( \omega \) is the dissipation rate per unit \( k \) and \((\sigma_k, \sigma_\omega, \beta, \beta^*, \kappa, \gamma)\) are the model constants. If \( \phi_1 \) and \( \phi_2 \) represent the set of constants used in the \( k-\omega \) and \( k-\epsilon \) models, respectively, then the blended set of constants \( \phi \) for the Menter BSL model are calculated as shown below:

\[
\phi = F_1 \phi_1 + (1 - F_1) \phi_2 \tag{2.58}
\]

where

\[
F_1 = \tanh \left( \arg_1^t \right) \tag{2.59}
\]

\[
\arg_1 = \min \left[ \max \left( \frac{\sqrt{k}}{0.09 \omega y_d}, \frac{500 \nu}{\omega y_d} \right), \frac{4 \bar{\rho} \sigma_{\omega 2} k}{CD_{k\omega} y_d^2} \right] \tag{2.60}
\]

\[
CD_{k\omega} = \max \left[ 2 \rho \sigma_{\omega 2} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 10^{-20} \right] \tag{2.61}
\]

\[
\mu_t = \frac{k}{\bar{\rho} \omega} \tag{2.62}
\]

where \( \nu \) is the kinematic viscosity and \( y_d \) is the distance to the nearest wall. The set of constants \( \phi_1 \) and \( \phi_2 \) are listed in Table 2.1.

**Menter SST Model**

For flows with adverse pressure gradients, full Reynolds-stress models have a superior performance compared to eddy-viscosity models. To incorporate this characteristic of the Reynolds-stress models into the framework of an eddy-viscosity model, Menter redefined the eddy viscosity from the BSL model as [67]:

\[
\mu_t = \frac{\bar{\rho} a_1 k}{\max (a_1 \omega; \Omega F_2)} \tag{2.63}
\]

where

\[
F_2 = \tanh \left( \arg_2^t \right) \tag{2.64}
\]
\[
\text{arg}_2 = \max \left(2 \sqrt{\frac{k}{0.09 \omega y_d}}, \frac{500 \nu}{y_d^3 \omega}\right)
\]  

where \( \Omega \) is the magnitude of vorticity. In the SST model, the set of constants to be used for the \( k - \omega \) model (\( \phi_1 \)) are shown in Table 2.1. The set of constants for the \( k - \epsilon \) model (\( \phi_2 \)), the conservation equations for \( k \) and \( \omega \), and the blending function (\( F_1 \)) are same as they were in the BSL model.

Table 2.1: Model constants for Menter BSL and SST turbulence models

<table>
<thead>
<tr>
<th>Constant</th>
<th>BSL (( \phi_1 ))</th>
<th>BSL (( \phi_2 ))</th>
<th>SST (( \phi_1 ))</th>
<th>SST (( \phi_2 ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_k )</td>
<td>0.5000</td>
<td>1.0000</td>
<td>0.8500</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \sigma_\omega )</td>
<td>0.5000</td>
<td>0.8560</td>
<td>0.5000</td>
<td>0.8560</td>
</tr>
<tr>
<td>( \beta )</td>
<td>0.0750</td>
<td>0.0828</td>
<td>0.0750</td>
<td>0.0828</td>
</tr>
<tr>
<td>( \beta^* )</td>
<td>0.0900</td>
<td>0.0900</td>
<td>0.0900</td>
<td>0.0900</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>0.5532</td>
<td>0.4404</td>
<td>0.5532</td>
<td>0.4404</td>
</tr>
</tbody>
</table>

2.2.3 Filtered Navier-Stokes Equations

The flow inside a scramjet is highly transient, which means it cannot be accurately approximated using a time-averaged set of equations. The straightforward choice is to solve the instantaneous Navier-Stokes equations by resolving all scales of turbulence. However, as mentioned before, this requires very fine meshes, which are impractical to deal with. Another choice is to compromise on the scales of turbulence one wishes to resolve, which is the fundamental philosophy of large-eddy simulation. In LES, the larger, geometry dependent scales of turbulence are resolved and the smaller turbulent scales, whose structures are universal, are modeled. The resolution of the geometry dependent turbulent scales helps in capturing the transient nature of the flow to a certain extent. The influences of the smaller (modeled) scales and the larger (resolved) scales of turbulence on the overall flow are uncoupled by using a three-dimensional spatial filtering operator,
shown in Equation 2.66.

\[
\bar{q}(x_1, x_2, x_3) = \int_{\xi_1} \int_{\xi_2} \int_{\xi_3} \left[ \prod_j G_j(x_j, \xi_j) \right] q(\xi_1, \xi_2, \xi_3) \, d\xi_1 \, d\xi_2 \, d\xi_3
\]  
(2.66)

The specific form of the spatial filtering operator used in the present work is shown in Equation 2.67, which is essentially a weighted local spatial average.

\[
G_j(x_j, \xi_j) = \begin{cases} 
\frac{1}{\Delta_j} & \text{if } |x_j - \xi_j| \leq \frac{\Delta_j}{2} \\
0 & \text{else}
\end{cases}
\]  
(2.67)

Similar to the RANS equations, to avoid dealing with large number of correlations, the filtered Navier-Stokes equations are expressed in terms of Favre-filtered quantities, which are density based spatially filtered quantities:

\[
\tilde{q} = \frac{\bar{p} \bar{q}}{\bar{q}}
\]  
(2.68)

The generic quantity \( q \) can then be expressed as a sum of the Favre-filtered quantity \( \tilde{q} \) and a density-weighted fluctuation \( q'' \):

\[
q = \tilde{q} + q''
\]  
(2.69)

Using the above notation, the Favre-filtered Navier-Stokes equations can be written as:

\[
\frac{\partial \bar{p}_s}{\partial t} + \frac{\partial}{\partial x_j} \left[ \bar{p}_s \left( \tilde{u}_j + \tilde{V}_{s,j} \right) + \rho \bar{Y}' Y''_{s,j} + \rho Y''_{s,s} \right] = \tilde{\omega}_s
\]  
(2.70)

\[
\frac{\partial (\bar{p} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} \left[ \bar{p} \tilde{u}_j \tilde{u}_i \right] = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \tau_{ij} - \rho \bar{u}_i'' \bar{u}_j'' \right]
\]  
(2.71)
\[
\frac{\partial}{\partial t} \left[ \sum_s \left( \tilde{p}_s \tilde{e}_s + \tilde{p}_s V_s^{"} e_s \right) \right] + \frac{1}{2} \tilde{\rho} \tilde{u}_i \tilde{u}_i + \frac{1}{2} \tilde{\rho} \tilde{u}_i \tilde{u}_j \frac{\partial}{\partial x_j} \left[ \tilde{u}_j \sum_s \left( \tilde{p}_s \tilde{h}_s \right) \right] + \sum_s \left( \tilde{Y}_s \rho u_j \tilde{h}_s + \tilde{h}_s \rho u_j \tilde{Y}_s + \tilde{\rho} u_j \tilde{Y}_s \tilde{h}_s \right) = \frac{\partial}{\partial x_j} \left[ \tilde{u}_j \tau_{ij} + \mu_t \delta_{ij} \right] = - \partial q_j \partial x_j + \frac{\partial}{\partial x_j} \left[ \tilde{\rho} \tilde{Y}_s \tilde{V}_{s,j} \right] \frac{\partial \tilde{T}}{\partial x_j} (2.72)
\]

where the subgrid correlations are highlighted in green. These correlations, which account for the subgrid species diffusion, subgrid stress, and subgrid heat flux, are modeled in the same manner as the turbulent terms were modeled for the RANS equations.

**Subgrid turbulent species diffusion:**

\[
\rho Y_s^{\"} u_j \equiv p_s V_s^{S} = - \frac{\mu_t}{S_c} \frac{\partial \tilde{Y}_s}{\partial x_j} (2.73)
\]

**Subgrid stress tensor (modeled):**

\[
- \rho u_i \tilde{u}_j \equiv \tau_{ij}^S = \mu_t \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu_t \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} - \frac{2}{3} \rho k \delta_{ij} (2.74)
\]

where $\mu_t$ is the subgrid eddy viscosity, which is modeled as described in §2.2.4. Also, the term $\frac{2}{3} \rho k \delta_{ij}$ is absorbed into the effective pressure $\tilde{p}$.

**Subgrid scale heat flux (modeled):**

\[
\sum_s \tilde{Y}_s \rho \tilde{h}_s \tilde{u}_j = q_j^S = - \frac{\mu_t}{\text{Pr}_t} \left( \sum_s \tilde{Y}_s \tilde{c}_{p,s} \right) \frac{\partial \tilde{T}}{\partial x_j} (2.75)
\]

where $\text{Pr}_t$ is the turbulent Prandtl number, which is set to 0.9 in the present work.

**Energy transport due to subgrid turbulent diffusion (modeled):**

\[
\sum_s \tilde{h}_s \rho \tilde{u}_j \tilde{Y}_s^{\"} \equiv \sum_s \tilde{p}_s \tilde{h}_s V_{s,j}^S (2.76)
\]
where \( V_{s,j} \) is calculated using Equation 2.73. Removing the neglected terms and replacing the above terms with their equivalent terms results in the following set of equations:

\[
\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho_s \left( \tilde{u}_j + \tilde{V}_{s,j} \right) + \rho_s V_{s,j} \right] = \tilde{\omega}_s \tag{2.77}
\]

\[
\frac{\partial (\rho \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho \tilde{u}_j \tilde{u}_i \right] = - \frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \tau_{ij} - \tau_{ij}^s \right] \tag{2.78}
\]

\[
\frac{\partial}{\partial t} \left[ \sum_s \rho_s \tilde{e}_s + \frac{1}{2} \rho \tilde{u}_i \tilde{u}_i \right] + \frac{\partial}{\partial x_j} \left[ \tilde{u}_j \left( \sum_s \rho_s \tilde{h}_s + \frac{1}{2} \rho \tilde{u}_i \tilde{u}_i \right) \right] = - \frac{\partial}{\partial x_j} \left[ q_j + q_j^s \right] + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \left( \tau_{ij} + \tau_{ij}^s \right) \right] - \frac{\partial}{\partial x_j} \left[ \sum_s \rho_s \tilde{h}_s \left( \tilde{V}_{s,j} + V_{s,j}^s \right) \right] \tag{2.79}
\]

### 2.2.4 Subgrid Closure for Eddy Viscosity

The subgrid eddy viscosity, which is used to model \( \tau_{ij}^s \) and \( q_j^s \), is calculated using a model developed by Lenormand et al. [68]:

\[
\mu_t = \rho C_M S^{\frac{1}{2}} \left( q_c^2 \right)^{\frac{1}{4}} \Delta^{\frac{3}{2}}, \quad C_M = 0.06 \tag{2.80}
\]

\[
\Delta = \sqrt{\Delta_x \Delta_y \Delta_z} \tag{2.81}
\]

where the strain rate \( S \) and subgrid kinetic energy \( q_c \) are given by:

\[
S = \left[ \frac{\partial \tilde{u}_i}{\partial x_j} \frac{\partial \tilde{u}_j}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{2}{3} \left( \frac{\partial \tilde{u}_i}{\partial x_i} \right)^2 \right]^{\frac{1}{2}} \tag{2.82}
\]

\[
q_c^2 = \frac{1}{2} \left( \tilde{u}_k - \tilde{u}_k \right)^2 \tag{2.83}
\]

The filter operation used in the above equation on a generic quantity is defined as:

\[
\tilde{q}_{i,j,k} = \frac{1}{2} q_{i,j,k} + \frac{1}{12} \left( q_{i+1,j,k} + q_{i-1,j,k} + q_{i,j+1,k} + q_{i,j-1,k} + q_{i,j,k+1} + q_{i,j,k-1} \right) \tag{2.84}
\]
2.2.5 Hybrid LES/RANS Model

Using LES to resolve all the relevant scales inside a turbulent boundary layer for a high Reynolds number flow is a computationally expensive task. To reduce the computational cost for LES, the turbulence inside the boundary layer (or a fraction of the boundary layer) is modeled using a RANS turbulence model, and an LES subgrid model is used everywhere else. This transition from \( \mu_{t,RANS} \) to \( \mu_{t,sgs} \) is made using a blending function \( \Gamma \):

\[
\mu_t = [(1 - \Gamma) \mu_{t,sgs} + \Gamma \mu_{t,RANS}]
\] (2.85)

In the present work, two different blending functions are used, one for the DLR combustor and another for the UVa combustors (Configurations A and E).

**DLR Combustor: Zonal Model**

The strengths and positions of various shock-boundary layer interactions play a crucial role in the prediction of shear layer development for this experiment, as reflected shocks from the walls traverse the mixing layer and alter its properties. To completely isolate wall-layer effects from the combustion zone, a zonal approach that utilizes Menter’s \( k - \omega \) model \[67\] near solid surfaces is employed. In all other regions, an LES subgrid model proposed by Lenormand *et al.* \[68\] is used, which is shown in Equation 2.80. The RANS model is blended with the LES subgrid model using the blending function shown in Equation 2.86.

\[
\Gamma = \max (\Gamma_1, \Gamma_2, \ldots, \Gamma_i)
\] (2.86)

In the above equation, \( \Gamma_i \) is calculated as shown in Equation 2.87.

\[
\Gamma_i = \frac{1}{2} \left( 1 + \tanh \left( \frac{l_i - y_{d,i}}{2 \times 10^{-4} \text{m}} \right) \right)
\] (2.87)

where \( l_i \) is the maximum boundary layer thickness along the \( i^{th} \) wall (assumed to be equal to a constant value of 0.0025 m for all the walls to ensure that the RANS model is used over the entire thickness of the boundary layer) and \( y_{d,i} \) is the distance of the cell from the \( i^{th} \) wall (measured in meters). More explanation as to why this model is used for the DLR combustor will be discussed in §5.1.4.
UVa Combustors: Dynamic Model

The blending function $\Gamma$ used in the simulations of the Configurations A and E of UVa’s SCF is calculated as shown in Equation 2.88 [69].

$$\Gamma = \frac{1}{2} \left(1 - \tanh \left[15 \left(\frac{1}{\lambda_N^2} - 1\right)\right]\right) \quad (2.88)$$

where $\lambda_N$, which ensures that the transition from the RANS to LES model is made as the boundary layer shifts from its logarithmic to its wake-like structure, is calculated as shown in Equation 2.89.

$$\lambda_N = \frac{l_{outer}}{l_{inner}} = C_N \sqrt{\frac{10\nu \bar{\omega} + \bar{k} + \bar{k}_R}{C_\mu^2 \bar{\omega}(\kappa y_d)^2}} \quad (2.89)$$

In Equation 2.89, $\bar{k}$ is the ensemble-averaged modeled turbulence kinetic energy, $\bar{k}_R$ is the ensemble-averaged resolved turbulence kinetic energy, $\omega$ and $\bar{\omega}$ are instantaneous and ensemble-averaged modeled turbulence frequencies, $\nu$ is the kinematic viscosity, $C_\mu = 0.09$, $C_N = 1.5$, $\kappa = 0.41$ is the Von Kármán constant, and $y_d$ is the distance to the nearest wall.

### 2.2.6 Subgrid Closures for Filtered Species Production Rates

As non-premixed combustion is necessarily preceded by macro- and micro-mixing, it is generally accepted that some type of subgrid-scale model for micro-mixing and the effects of unresolved fluctuations on the filtered species production rates ($\dot{\omega}(\rho_s, T)$) is necessary. The exact form of this model and the range of influence that it must have as a function of the chosen mesh resolution is a matter of debate, and as yet, no clear consensus has emerged. In the present work, different finite-rate chemistry subgrid closures are used to calculate the filtered species production rates. These closures are described below:
Laminar Chemistry Closure

The filtered species production rate can be calculated using a ‘laminar chemistry’ subgrid closure, which is shown in Equation 2.90.

\[
\dot{\omega}_s (\rho_s, T) \approx \dot{\omega}_s (\bar{\rho}, \tilde{T}) = \dot{\omega}_{s, \text{lam}} \quad (2.90)
\]

This model neglects the effects of subgrid fluctuations in species densities and temperature on the filtered species production rates. It also assumes that the entire fluid within a cell volume is well mixed, which might not be the case.

PaSR(0) Closure

The PaSR(0) closure aims at modeling the ‘un-mixedness’ of the mixture within a cell volume. In other words, the idea is that small-scale mixing must precede reactions, and if the mixing rate is slow enough, reactions must ‘wait’ to commence, and this should limit the species production rates. In this closure, the filtered species production rate is modeled as shown in Equation 2.91.

\[
\dot{\omega}_s (\rho_s, T) \approx f \dot{\omega}_s (\bar{\rho}, \tilde{T}) = f \dot{\omega}_{s, \text{lam}} \quad (2.91)
\]

where

\[
f = \frac{\bar{\rho}}{\bar{\rho} + c_1 t_{\text{sgs}} \max \left( \left| \dot{\omega}^+ (\bar{\rho}, \tilde{T}) \right|, \left| \dot{\omega}^- (\bar{\rho}, \tilde{T}) \right| \right)} \quad (2.92)
\]

Here, \(f\) represents the ratio: \(\frac{t_{\text{chem}}}{t_{\text{chem}} + c_1 t_{\text{sgs}}}\), where \(t_{\text{chem}}\) and \(t_{\text{sgs}}\) are the chemistry and mixing time-scales, respectively. Meaning, if the mixing time-scale \(t_{\text{sgs}}\) is much larger than the chemistry time-scale \(t_{\text{chem}}\), then the value of \(f\) is lesser than one and the PaSR(0) closure will have the effect of decreasing the species production rates predicted by the ‘laminar chemistry’ assumption. In other words, within a finite volume in space and in a given amount of time, the overall production of species due to chemical reactions should be limited by the amount of time the fluid spends in forming a well mixed mixture. In Equation 2.92, \(c_1\) is a model constant and the mixing time-scale \(t_{\text{sgs}}\) is defined as:

\[
t_{\text{sgs}} = \frac{\Delta}{\max \left( \frac{\nu}{\kappa}, u_{\text{sgs}} \right)} \quad \text{and} \quad u_{\text{sgs}} = \sqrt{\frac{2}{3} \left[ \tilde{u}_1^2 - \tilde{u}_1 + \tilde{u}_2^2 - \tilde{u}_2 + \tilde{u}_3^2 - \tilde{u}_3 \right]} \quad (2.93)
\]
where $\nu$ is the kinematic viscosity and $\Delta$ is the filter-width. The filtering operation ($\hat{\cdot}$) is performed using Equation 2.84. The formulation of the terms $\left| \dot{\omega}^+ (\bar{\rho}_s, \bar{T}) \right|$ and $\left| \dot{\omega}^- (\bar{\rho}_s, \bar{T}) \right|$, used in Equation 2.92, is described below. First, the net rate of the $k^{th}$ reaction $R_k$ is written as the sum of the forward and backward reaction rates, $R_k^+$ and $R_k^-$, respectively.

$$R_k = R_k^+ + R_k^-$$ (2.94)

where

$$R_k^+ = k_f,k \prod_k \left( \frac{\rho_s}{M_s} \right)^{\nu'_{s,k}} \text{ and } R_k^- = -k_b,k \prod_k \left( \frac{\rho_s}{M_s} \right)^{\nu''_{s,k}}$$ (2.95)

Using $R_k^+$ and $R_k^-$, the species production rate can be written as

$$\dot{\omega}_s(\rho_s, T) = \sum_k \left( \nu''_{s,k} - \nu'_{s,k} \right) \left[ R_k^+ - R_k^- \right] = \dot{\omega}_s^+ - \dot{\omega}_s^-$$ (2.96)

where

$$\dot{\omega}_s^+ = \sum_k \left[ \nu''_{s,k} R_k^+ + \nu'_{s,k} R_k^- \right] \text{ and } \dot{\omega}_s^- = \sum_k \left[ \nu''_{s,k} R_k^- + \nu'_{s,k} R_k^+ \right]$$ (2.97)

Finally, $\left| \dot{\omega}^+ (\bar{\rho}_s, \bar{T}) \right|$ and $\left| \dot{\omega}^- (\bar{\rho}_s, \bar{T}) \right|$, which are the $L^2$ norms of $\dot{\omega}_s^+$ and $\dot{\omega}_s^-$, respectively, are defined as

$$\left| \dot{\omega}^+ (\bar{\rho}_s, \bar{T}) \right| = \left( \sum_s (\dot{\omega}_s^+)^2 \right)^{\frac{1}{2}} \text{ and } \left| \dot{\omega}^- (\bar{\rho}_s, \bar{T}) \right| = \left( \sum_s (\dot{\omega}_s^-)^2 \right)^{\frac{1}{2}}$$ (2.98)

**PaSR(1) Closure**

In the PaSR(1) subgrid closure, it is assumed that each computational mesh cell consists of fine-scale (Kolmogorov scale) structures and coarser structures (Figure 2.1) [11, 70, 71, 72], and the average filtered species production rate is then defined as a sum of the reaction rates within these structures:

$$\bar{\omega}_s(\rho_s, T) = \gamma^* \dot{\omega}_s(\rho_s^*, T^*) + (1 - \gamma^*) \dot{\omega}_s(\rho_s^0, T^0)$$ (2.99)

where $\gamma^*$ is the volume fraction of fine-scale structures, and the terms denoted with * and 0 correspond to fine-scale and coarser structures, respectively. Thermodynamic properties of the fine-scale structures are governed by NS mass and one energy conservation equations.
Figure 2.1: PaSR(1): Cell-volume containing reacting fine-scale structures embedded in reacting coarser structures.
Mass conservation of species $s$ in fine-scale structures:

$$
\Omega^* \frac{\partial (\rho^*_s)}{\partial t} + \int_A \rho^*_s \gamma^*_s u_j . n_j dA + \int_A^* \rho_s V_{s,j} . n_j dA^* = \Omega^* \dot{\omega}_s (\rho^*_s, T^*)
$$

Energy conservation in fine-scale structures:

$$
\Omega^* \frac{\partial [\sum_s \rho^*_s h_s (T^*)]}{\partial t} + \int_A \sum_s \rho_s h_s (T^*) \gamma^*_s u_j . n_j dA

+ \int_A^* \left[ \left( \sum_s \rho_s (T) V_{s,j} \right) + q_j \right] . n_j dA^* = 0
$$

where $\Omega^*$ represents the actual volume occupied by the fine-scale structures. Terms I and III represent change in mass and energy of the fine-scale structures within a cell-volume due to convection; terms II and IV represent the exchange of mass and energy between fine-scale and coarser structures. While terms I and III can be evaluated by performing the surface integral over the cell-surface, terms II and IV require modeling, as the exact shape and surface area of the interface between fine-scale and coarser structures are not known. To this end, the above two equations are rewritten as:

$$
\Omega^* \frac{\partial (\rho^*_s)}{\partial t} + \int_A \rho^*_s \gamma^*_s u_j . n_j dA + \rho_s \overline{V_{s,j}} . n_j dA^* = \Omega^* \dot{\omega}_s (\rho^*_s, T^*)
$$

$$
\Omega^* \frac{\partial [\sum_s \rho^*_s h_s (T^*)]}{\partial t} + \int_A \sum_s \rho_s h_s (T^*) \gamma^*_s u_j . n_j dA +

\left[ \left( \sum_s \rho_s (T) V_{s,j} \right) + q_j . n_j \right] A^* = 0
$$

where the overbars represent the average flux evaluated over the interface between the fine-scale structures and the remainder of fluid in the volume. Substituting a Fickian
diffusion model for $V_{s,j}$ and Fourier’s law for $q_j$, we have that

$$
q_j = -k \frac{\partial T}{\partial x_j} \approx -k_I \frac{(T^0 - T^*)}{\Delta s} n_j 
$$

(2.104)

$$
\rho_s V_{s,j} = -\rho D \frac{\partial Y_s}{\partial x_j} \approx \rho_I D_I \frac{Y_s^0 - Y_s^*}{\Delta s} n_j 
$$

(2.105)

$$
\sum_s \rho_s h_s(T) V_{s,j} = -\rho D \sum_s h_s(T) \frac{\partial Y_s}{\partial x_j} \approx -\rho_I D_I \sum_s h_s(T_I) \frac{Y_s^0 - Y_s^*}{\Delta s} n_j 
$$

(2.106)

where $\Delta s$ is a diffusion length scale and the terms with the subscript $I$ correspond to values of various quantities at the interface between the fine-scale and coarse structures.

With these models, the subgrid balance equations become:

$$
\Omega^* \frac{\partial (\rho^*_s)}{\partial t} + \int_A \rho^*_s \gamma_s^* u_j, n_j dA - \rho_I D_I \frac{Y_s^0 - Y_s^*}{\Delta s} A^* = \Omega^* \dot{\omega}_s (\rho^*_s, T^*) 
$$

(2.107)

$$
\Omega^* \frac{\partial [\sum_s \rho^*_s h_s(T^*)]}{\partial t} + \int_A \sum_s \rho^*_s h_s(T^*) \gamma_s^* u_j, n_j dA - k_I \frac{(T^0 - T^*)}{\Delta s} A^* \\
- \rho_I D_I \sum_s h_s(T_I) \frac{Y_s^0 - Y_s^*}{\Delta s} A^* = 0 
$$

(2.108)

An alternative form of the above pair of equations places the density inside the Fickian diffusion model, as shown below:

$$
\Omega^* \frac{\partial (\rho^*_s)}{\partial t} + \int_A \rho^*_s \gamma_s^* u_j, n_j dA - D_I \frac{\rho_s^0 - \rho_s^*}{\Delta s} A^* = \Omega^* \dot{\omega}_s (\rho^*_s, T^*) 
$$

(2.109)

$$
\Omega^* \frac{\partial [\sum_s \rho^*_s h_s(T^*)]}{\partial t} + \int_A \sum_s \rho^*_s h_s(T^*) \gamma_s^* u_j, n_j dA - k_I \frac{(T^0 - T^*)}{\Delta s} A^* \\
- D_I \sum_s h_s(T_I) \frac{\rho_s^0 - \rho_s^*}{\Delta s} A^* = 0 
$$

(2.110)
Defining $\gamma^* = \frac{\Omega^*}{\Delta s}$ as the volume fraction of fine-scale structures, we have that

$$\bar{Y}_s = \gamma^* Y_s^* + (1 - \gamma^*) Y_s^0, \quad \bar{p}_s = \gamma^* \rho_s^* + (1 - \gamma^*) \rho_s^0, \quad \bar{T} = \gamma^* T^* + (1 - \gamma^*) T^0 \tag{2.111}$$

where the values on the left-hand sides of each expression are those representative of the filtered data extracted by solving the filtered Navier-Stokes equations. Rewriting Equations 2.111:

$$Y_s^0 - Y_s^* = \frac{\bar{Y}_s - Y_s^*}{1 - \gamma^*}, \quad \rho_s^0 - \rho_s^* = \frac{\bar{p}_s - \rho_s^*}{1 - \gamma^*}, \quad T^0 - T^* = \frac{\bar{T} - T^*}{1 - \gamma^*} \tag{2.112}$$

Substituting the relations from Equation 2.112 in Equations 2.109 and 2.110, and rearranging, we get:

$$(1 - \gamma^*) \left( \frac{\partial (\rho_s^* \gamma^*)}{\partial t} + \frac{1}{\Omega^*} \int_A \rho_s^* \gamma^* u_j . n_j dA \right) - D_I \frac{A^*}{\Omega^* \Delta s} (\bar{p}_s - \rho_s^*) = (1 - \gamma^*) \omega_s (\rho_s^*, T^*) \tag{2.113}$$

$$(1 - \gamma^*) \left( \frac{\partial \left( \sum_s \rho_s^* h_s (T^*) \right)}{\partial t} + \frac{1}{\Omega^*} \int_A \sum_s \rho_s^* h_s (T^*) \gamma^* u_j . n_j dA \right) - k_I \frac{A^*}{\Omega^* \Delta s} \left( \bar{T} - T^* \right) - D_I \frac{A^*}{\Omega^* \Delta s} \sum_s h_s (T_I) (\bar{p}_s - \rho_s^*) = 0 \tag{2.114}$$

It now remains to define the interface transport coefficients $D_I$ and $k_I$, the volume fraction occupied by fine structures $\gamma^*$, and the quantity $\frac{A^*}{\Omega^* \Delta s}$, where $A^*$ is the surface area of the fine structures, $\Omega^*$ is the volume occupied by fine structures, and $\Delta s$ is a diffusion length scale. $D_I$ and $k_I$ are calculated by associating these interface values with the average state within a cell:

$$D_I = \frac{1}{Sc} \frac{\mu_{mix,I}}{\rho_I} = \frac{1}{Sc} \frac{\bar{\mu}_{mix}}{\bar{\rho}} \tag{2.115}$$

$$k_I = \frac{1}{Pr} \frac{\mu_{mix,I} c_p, mix,I}{c_p, mix} = \frac{1}{Pr} \frac{\bar{\mu}_{mix}}{\bar{c}_p, mix} \tag{2.116}$$
Substituting the above expressions for \( D_I \) and \( k_I \) in Equations 2.113 and 2.114:

\[
(1 - \gamma^*) \left( \frac{\partial (\rho^*_s)}{\partial t} + \frac{1}{\Omega^*} \int_A \rho^*_s \gamma^*_s u_j, n_j dA \right) \quad \frac{1}{Sc} \frac{\bar{p}_{mix}}{\bar{p}} \frac{A^*}{\Omega^*} (\bar{p}_s - \rho^*_s) = (1 - \gamma^*) \dot{\omega}_s (\rho^*_s, T^*) \quad (2.117)
\]

\[
(1 - \gamma^*) \left( \frac{\partial \left( \sum_s \rho^*_s h_s(T^*) \right)}{\partial t} + \frac{1}{\Omega^*} \int_A \sum_s \rho^*_s h_s(T^*) \gamma^*_s u_j, n_j dA \right) \quad \frac{1}{Pr} \rho Sc \tilde{C}_{p,mix} (\tilde{T} - T^*) - \frac{1}{t_m} \sum_s h_s(T_1) (\bar{p}_s - \rho^*_s) = 0 \quad (2.118)
\]

The term \( \frac{1}{(1 - \gamma^*) \frac{\bar{p}_{mix}}{\bar{p}} \frac{A^*}{\Omega^* \Delta s}} \) can be replaced with a time-scale \( t_m \), which is characteristic of the diffusion-driven exchange of mass and energy between the fine-scale structures and the remainder. This replacement results in Equations 2.119 and 2.120.

\[
(1 - \gamma^*) \left( \frac{\partial (\rho^*_s)}{\partial t} + \frac{1}{\Omega^*} \int_A \rho^*_s \gamma^*_s u_j, n_j dA \right) - \frac{1}{t_m} (\bar{p}_s - \rho^*_s) = (1 - \gamma^*) \dot{\omega}_s (\rho^*_s, T^*) \quad (2.119)
\]

\[
(1 - \gamma^*) \left( \frac{\partial \left( \sum_s \rho^*_s h_s(T^*) \right)}{\partial t} + \frac{1}{\Omega^*} \int_A \sum_s \rho^*_s h_s(T^*) \gamma^*_s u_j, n_j dA \right) \quad - \frac{1}{Pr} \tilde{C}_{p,mix} (\tilde{T} - T^*) - \frac{1}{t_m} \sum_s h_s(T_1) (\bar{p}_s - \rho^*_s) = 0 \quad (2.120)
\]

For closure, the volume fraction of fine-scale structures \( \gamma^* \) and time-scale \( t_m \) need to be defined. Different models have been proposed to define \( \gamma^* \) and \( t_m \), three of which are described below:

1. Giacomazzi et al. [13]:

\[
t_m = Sc \frac{l_k^2}{\bar{p}_{mix} \bar{p}} \quad (2.121)
\]
\[ \gamma^* = \left( \pi^{-\frac{1}{2}} Re^{-\frac{1}{4}} \right)^{\log(\pi) \log(a^{1/6} Re^{1/2})} \]  

(2.122)

where \( l_k = \Delta \pi^{-\frac{1}{2}} Re^{\frac{1}{4}} \), \( Re_{\Delta} = \frac{Re}{\rho_{mix}} \), and \( u_{sgs} \) is the root-mean-square (rms) of the subgrid velocity fluctuations. It is important to mention that in their model, Giacomazzi et al. [13] assume that each cell is comprised of reacting fine-scale structures embedded in the non-reacting coarser structures. This assumption differs from the assumption made in the current model (termed PaSR(1)): each cell is comprised of reacting fine-scale structures embedded in reacting coarser structures, and the rates at which reactions occur in the fine-scale and coarser structures are different. This assumption is similar to the one made by Fureby et al. [73, 12] and in the Eddy Dissipation Concept [74].

2. Fureby et al. [73, 12]:

\[ t_m = \Delta \frac{Re^{\frac{1}{4}}}{u_{sgs}} \]  

(2.123)

\[ \gamma^* = \frac{t_c}{t_c + t_m} \]  

(2.124)

where \( t_c = \frac{\delta_u}{s_u} \), with \( \delta_u \) and \( s_u \) being the laminar flame thickness and laminar flame speed, respectively. For hydrogen-air combustion at stoichiometric conditions, \( \delta_u \approx 0.5 \text{ mm} \) and \( s \approx 2 \text{ m/s} \).

3. Eddy Dissipation Concept (EDC) [74]:

\[ t_m = 0.9075 \Delta \frac{Re^{\frac{1}{4}}}{u_{sgs}} \]  

(2.125)

\[ \gamma^* = 0.876 Re^{\frac{3}{4}} \]  

(2.126)

Equations 2.119 and 2.120 are solved in tandem with the main flow equations. The preceding development is related to the eddy-dissipation and PaSR models used by Fureby and co-workers [74, 73, 12] but differs in its inclusion of convective transport of fine-scale structures and its use of alternative expressions for the subgrid mixing time-scale and the volume fraction of fine-scale structures. A comparison of the present expressions with those in the literature is presented in §6.4. In the present work, the time-scale and fine-scale volume fraction definitions of Giacomazzi et al. [13] are used to close the system of equations defined by Equations 2.119 and 2.120.
\textbf{PaSR/Scale-Similarity Model (PaSR(SS))}

In this model, the time-scale ratio used in the PaSR(0) model is defined in terms of information obtained from test-filtering the grid-scale data as shown in Equation 2.84. The intent is to calculate a measure of ‘un-mixedness’ in the solution based on the test-filtered data and to utilize it to model the unknown degree of ‘un-mixedness’ found at the subgrid-scale level. The model definition considered in this work is as follows:

\[
\dot{\omega}_s(\rho_s, T) = \min \left( c_3, c_1 \left\| \dot{\omega}_{s,\text{lam}} \right\| + \frac{c_2 \mu}{\Delta^2} \right) \dot{\omega}_{s,\text{lam}}
\]

(2.127)

In contrast to the PaSR(0) model, this formulation can allow augmentation of the species production rates. An additional model constant \(c_3\) (set to 2.0) is used to limit the degree to which this can occur. Also, to avoid numerical difficulties where the species production rates are very small, a factor of \(c_2 \mu/\Delta^2\) (with \(c_2\) equal to 0.1) is added to the numerator and denominator of the ‘un-mixedness’ term.

\textbf{Scale-Similarity Model (SS)}

Motivated by the relative success of scale-similarity closures for simpler SGS terms, Desjardin and Frankel [75] developed several such closures for the chemical production terms. While these were shown to correlate DNS data relatively well, they were only tested for 2D shear layers with single-step reactions. A representative scale-similarity closure is

\[
\dot{\bar{\omega}}_s(\rho_s, T) = \dot{\omega}_{s,\text{lam}} + c_1 \left[ \dot{\omega}_{s,\text{lam}} - \dot{\omega}_s(\tilde{\rho}_s, \tilde{T}) \right]
\]

(2.128)

where the filtering operation (\(\tilde{\cdot}\)) is performed as shown in Equation 2.84. In all of the aforementioned models, the scaling constant must be determined. Procedures for estimating this constant and assessing the performance of each model through a \textit{a priori} analyses are discussed later in the paper.
Chapter 3

Numerical Methods

To numerically solve the Reynolds-averaged or filtered Navier-Stokes equations, the time and spatial derivatives must be discretized; the discretized set of equations must then be solved using a time-integration technique. In this chapter, these techniques along with other methods used to improve the accuracy and fidelity of the simulations are presented. The first step in this process is to write the Reynolds-averaged or filtered Navier-Stokes equations in vector form:

$$\frac{\partial U}{\partial t} + \frac{\partial F_j}{\partial x_j} + \frac{\partial G_j}{\partial t} = S$$

Conservative variable vector:

$$U = \begin{bmatrix} \bar{\rho}_1 \\ . \\ . \\ \bar{\rho}_{NS} \\ \bar{\rho}_{u1} \\ \bar{\rho}_{u2} \\ \bar{\rho}_{u3} \\ \sum_s \bar{p}_s e_s + \frac{1}{2} \bar{p}_{u1} \bar{u}_1 + \bar{p} k \\ \bar{p} k \\ \bar{p} \omega \end{bmatrix}$$
Inviscid flux vector:

\[
F_j = \begin{bmatrix}
\tilde{p}_1 \left( \tilde{u}_j + \tilde{V}_{1,j} \right) \\
\vdots \\
\tilde{p}_{NS} \left( \tilde{u}_j + \tilde{V}_{NS,j} \right) \\
\tilde{p}_{1} \tilde{u}_j + \delta_{1,j} \tilde{p} \\
\tilde{p}_{2} \tilde{u}_j + \delta_{1,j} \tilde{p} \\
\tilde{p}_{3} \tilde{u}_j + \delta_{1,j} \tilde{p} \\
\tilde{u}_j \left( \sum_s \tilde{p}_s \tilde{h}_s + \frac{1}{2} \tilde{p}\tilde{u}_i \tilde{u}_i + \tilde{p} k \right) \\
\tilde{u}_j \tilde{p} k \\
\tilde{u}_j \tilde{p} \omega
\end{bmatrix}
\]  

(3.3)

Viscous flux vector:

\[
G_j = \begin{bmatrix}
0 \\
\vdots \\
0 \\
-\tau_{1j} - \tau_{1j}^t \\
-\tau_{2j} - \tau_{2j}^t \\
-\tau_{3j} - \tau_{3j}^t \\
\tilde{q}_j + \tilde{q}_j^t + \tilde{u}_i \left( \tau_{ij} + \tau_{ij}^t \right) + \sum_s \tilde{p}_s \tilde{h}_s \tilde{V}_{s,j} \\
- \left( \mu + \sigma_k \mu_t \right) \frac{\partial k}{\partial x_j} \\
- \left( \mu + \sigma_\omega \mu_t \right) \frac{\partial \omega}{\partial x_j}
\end{bmatrix}
\]  

(3.4)
Source vector:

\[
S = \begin{bmatrix}
\bar{\omega}_1 \\
. \\
. \\
\bar{\omega}_{NS} \\
0 \\
0 \\
0 \\
0 \\
\beta^* \rho \omega k + \tau^t_{ij} \frac{\partial \bar{u}_i}{\partial x_j} \\
-\beta^* \rho \omega^2 + \frac{\gamma}{\mu} \tau^t_{ij} \frac{\partial \bar{u}_i}{\partial x_j} + 2 (1 - F_1) \rho \sigma \omega^2 \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}
\end{bmatrix}
\tag{3.5}
\]

In a finite-volume approach, the above set of conservation equations is first integrated over the volume of a mesh cell \( V \):

\[
\int_V \left( \frac{\partial U}{\partial t} + \frac{\partial F_j}{\partial x_j} + \frac{\partial G_j}{\partial t} \right) dV = \int_S S dV \tag{3.6}
\]

Using the divergence theorem, the volume integrals of the inviscid and viscous fluxes can be written as integrals along the cell surface \( S \):

\[
\int_V \frac{\partial U}{\partial t} dV + \int_S F_j n_j dS + \int_S G_j n_j dS = \int_V S dV \tag{3.7}
\]

The above form of the conservation equations can be written in its discretized form as shown below:

\[
\frac{\Delta U}{\Delta t} \Omega_{CV} + \sum_{cell-faces} \left( (F_j + G_j)n_j \right)_f S_f = S \Omega_{CV} \tag{3.8}
\]

where \( \Omega_{CV} \) is the cell-volume and \( S_f \) is the area of the cell-face \( f \).

### 3.1 Inviscid Flux Discretization

The various derivatives appearing in Equation 3.7 can be discretized using a variety of differencing techniques. However, in fluid dynamics, it is essential that these techniques
take into account the direction of information transmission within the fluid, which is represented by the inviscid flux vector $\mathbf{F}_j$. For example, in a flow with zero fluid velocity, information travels from a point A in all directions in the form of characteristic waves, which travel at the local speed of sound. So, all locations upstream and downstream of point A will receive information about the local flow properties at point A. However, if the local flow speed at point A is supersonic, the characteristic waves cannot reach upstream locations. Which means, flow properties at an upstream location are not affected by the flow properties at point A. The technique used to discretize the inviscid flux vector should be capable of capturing this phenomenon.

In the present work, the inviscid fluxes are discretized using Edwards’ Low Diffusion Flux Splitting Scheme (LDFSS) [76], which accounts for information transmission at all flow speeds and is a variant of the standard van Leer Scheme [77]. In this scheme, the face-normal projection of the inviscid flux is first split into convective and pressure components:

$$n_j \mathbf{F}_j = (n_j \mathbf{F}_j)^c + (n_j \mathbf{F}_j)^p = \bar{\rho} n_j \tilde{u}_j \mathbf{E}^c + \bar{\rho} \mathbf{E}^p$$

where

$$\mathbf{E}^c = \begin{bmatrix} \tilde{Y}_1 \\ \vdots \\ \tilde{Y}_{NS} \\ \tilde{u}_1 \\ \tilde{u}_2 \\ \tilde{u}_3 \\ \left( \sum_s \tilde{Y}_s \tilde{h}_s + \frac{1}{2} \tilde{u}_i \tilde{u}_i + k \right) \\ k \\ \omega \end{bmatrix}$$

and

$$\mathbf{E}^p = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ n_1 \\ n_2 \\ n_3 \\ 0 \\ 0 \end{bmatrix}$$

The convective component at the cell face between cells $i$ and $i + 1$ (represented by $i + \frac{1}{2}$) is then expressed as:

$$(n_j F_j)_{i + \frac{1}{2}}^c = a_{i + \frac{1}{2}} \left[ \bar{\rho}_L C^+ E_L^c + \bar{\rho}_R C^- E_R^c \right]$$
where

\[ a_{i+\frac{1}{2}} = \frac{1}{2} (a_L + a_R) \]  
\[ C^+ = \alpha_L^+ (1 + \beta_L) M_L - \beta_L M^+ - M^+_{\frac{1}{2}} \]  
\[ C^- = \alpha_R^- (1 + \beta_R) M_R - \beta_R M^- - M^-_{\frac{1}{2}} \]  
\[ M^+_{\frac{1}{2}} = M_{\frac{1}{2}} \left[ \frac{2\bar{p}_R}{\bar{p}_R + \bar{p}_L} \right] - \delta \frac{\bar{p}_L - \bar{p}_R}{\bar{p}_L}, \delta = 2.0 \]  
\[ M^-_{\frac{1}{2}} = M_{\frac{1}{2}} \left[ \frac{2\bar{p}_L}{\bar{p}_R + \bar{p}_L} \right] - \delta \frac{\bar{p}_L - \bar{p}_R}{\bar{p}_R}, \delta = 2.0 \]  
\[ \alpha^{\pm}_{L/R} = \frac{1}{2} \left[ 1 \pm \text{sign} \left( M_{L/R} \right) \right] \]  
\[ \beta_{L/R} = - \max \left[ 0, 1 - \text{int} \left( |M_{L/R}| \right) \right] \]  
\[ M^\pm_{L,R} = \pm \frac{1}{4} \left[ M_{L,R} \pm 1 \right]^2 \]  
\[ M_{\frac{1}{2}} = \frac{1}{4} \beta_L \beta_R \left[ \sqrt{\frac{1}{2} (M^2_L + M^2_R)} - 1 \right] \]  
\[ M_{L/R} = \frac{1}{a_{i+\frac{1}{2}}} n_j \tilde{u}_{j,L/R} \]  

The pressure component at the \( i + \frac{1}{2} \) cell face is given by:

\[ (n_j F_j)^p_{i+\frac{1}{2}} = \mathbf{E}^p_{i+\frac{1}{2}} \left[ D^+_L \bar{p}_L + D^-_R \bar{p}_R \right] \]  

where

\[ D^\pm_{L/R} = \alpha^\pm_{L/R} \left[ 1 + \beta_{L/R} \right] - \beta_{L/R} P^\pm_{L/R} \]  
\[ P^\pm_{L/R} = \frac{1}{4} \left( M_{L/R} \pm 1 \right)^2 \left( 2 \mp M_{L/R} \right) \]  

### 3.2 Viscous Fluxes

The viscous fluxes are discretized using a simple second order central-differencing reconstruction about the cell interface.
3.3 Reconstruction Methods

In the LDFSS scheme, a simple approximation to the $L$ and $R$ states can be to use the data from the cell centers of $i$ and $i + 1$ cells. This approximation essentially assumes that fluid properties do not vary within the cell volume, which will result in first-order spatial accuracy for the inviscid fluxes. Extending the spatial accuracy of the inviscid fluxes will improve the capturing of the shock-waves and contact discontinuities. To this end, two different reconstruction schemes are used in the present work. In both schemes, a fourth-order averaging technique is first applied to the primitive variable vector $\mathbf{W} = [p, u, v, w, T, k, \omega]$ to obtain initial left- and right-states at a cell interface. These initial left- and right-states (denoted with the superscript $A$) are calculated as shown in Equation 3.25, which yields fourth order spatial accuracy on uniform meshes.

$$W_{L,i+\frac{1}{2}}^A = \frac{7}{12} (W_i + W_{i+1}) - \frac{1}{12} (W_{i+2} + W_{i-1})$$

The reconstruction is then made monotone by using Total Variation Diminishing (TVD) [78] or Piecewise Parabolic Method (PPM) [79] reconstruction schemes, resulting in the final monotonicity preserving left- and right-states (denoted with superscript $M$).

3.3.1 Total Variation Diminishing (TVD) Scheme

The TVD scheme enforces monotonicity of the data using a minmod operator:

$$W_{L,i+\frac{1}{2}}^M = W_i + \frac{1}{2} \text{minmod} (W_{i+1} - W_i, W_i - W_{i-1})$$

$$W_{R,i+\frac{1}{2}}^M = W_{i+1} - \frac{1}{2} \text{minmod} (W_{i+2} - W_{i+1}, W_{i+1} - W_i)$$
3.3.2 Piecewise Parabolic Method (PPM)

In the PPM scheme, monotonicity is enforced by resetting the $L$ and $R$ states of each cell using the following algorithm:

$$W_{L,i+\frac{1}{2}}^M = W_{L,i+\frac{1}{2}}^A$$
$$W_{R,i-\frac{1}{2}}^M = W_{R,i-\frac{1}{2}}^A$$

if $\text{sgn} \left[ \left( W_{L,i+\frac{1}{2}}^A - W_i \right) \left( W_i - W_{R,i-\frac{1}{2}}^A \right) \right] = -1$, then

$$W_{L,i+\frac{1}{2}}^M = W_{R,i-\frac{1}{2}}^M = W_i$$

else

$$C = W_{L,i+\frac{1}{2}}^A - W_{R,i-\frac{1}{2}}^A; \quad D = 6 \left[ W_i - \frac{1}{2} \left( W_{L,i+\frac{1}{2}}^A + W_{R,i-\frac{1}{2}}^A \right) \right]$$

if $(D \times C > C \times C)$ then

$$W_{R,i-\frac{1}{2}}^M = 3W_i - 2W_{L,i+\frac{1}{2}}^A$$

elseif $(-C \times C > D \times C)$ then

$$W_{L,i+\frac{1}{2}}^M = 3W_i - 2W_{R,i-\frac{1}{2}}^A$$

end if

end if

This enforcement of monotonicity adds numerical dissipation proportional to the difference between the final and initial states. While this addition of numerical dissipation is good for regions capturing strong shocks, it has a negative effect on the performance of the scheme in the regions where small-scale turbulent structures are to be captured. To address this issue, the initial left- and right-states (fourth order accurate) are blended with the final monotonicity-preserving states (states with added dissipation) using the vorticity / divergence function proposed by Ducros et al. [80], defined at a mesh cell as shown in Equation 3.30.

$$f = \frac{\left( \nabla \vec{V} \right)^2}{\left( \nabla \cdot \vec{V} \right)^2 + \mid \omega \mid^2 + \epsilon^2}, \quad \epsilon = 1 \times 10^{-8}V_{\infty}/\max (\Delta x, \Delta y, \Delta z)$$ (3.30)
where $\omega$ is the vorticity; $V_\infty$ is the freestream velocity; and $\Delta x$, $\Delta y$, and $\Delta z$ are the average cell spacings on the entire grid in the $x$-, $y$-, and $z$-directions, respectively, calculated as shown below:

$$
\Delta x, y, z = \sum_{i=1}^{N_{\text{Cells}}} \frac{\Delta x_i, y_i, z_i}{N_{\text{Cells}}}
$$

(3.31)

The blended left- and right-states are calculated as shown in Equations 3.32 and 3.33 using the blending function $f$.

$$
W_{L,i+\frac{1}{2}} = W_{A,L,i+\frac{1}{2}} + \max(f_i, f_{i+1}) \left( W_{M,L,i+\frac{1}{2}} - W_{A,L,i+\frac{1}{2}} \right)
$$

(3.32)

$$
W_{R,i+\frac{1}{2}} = W_{A,R,i+\frac{1}{2}} + \max(f_i, f_{i+1}) \left( W_{M,R,i+\frac{1}{2}} - W_{A,R,i+\frac{1}{2}} \right)
$$

(3.33)

These blended left- and right-states are then given as input to the LDFSS scheme to calculate the interface inviscid fluxes.

### 3.4 Time Integration

#### 3.4.1 RANS and LES Equations

The final discretized form of the RANS or LES equations can be written as:

$$
\frac{\Delta U}{\Delta t} \Omega_{CV} + \sum_{\text{cell-faces}} (E_j n_j)_f S_f = S \Omega_{CV}
$$

(3.34)

where

$$
E_j = F_j + G_j
$$

(3.35)

Defining the steady residual $R_s$ as:

$$
R_s = \sum_{\text{cell-faces}} (E_j n_j)_f S_f - S \Omega_{CV}
$$

(3.36)

The above set of equations can be discretized explicitly in time by evaluating the steady residual $R_s$ using the data from the current time-step $n$. By doing this, the conserved variable vector at the $(n+1)^{th}$ time-step can be evaluated in a straightforward manner.
However, an explicit formulation will impose severe restrictions on the size of the time-step that can be used. In other words, the system will be numerically stable only for very small time-steps, which increases the overall computational cost at least by a couple of orders of magnitude. The reason for the numerical instability of an explicit formulation is the large variation in the time-scales characteristic of the chemical kinetics and the fluid flow, which results in a very strong coupling between reactive kinetics and compressible fluid dynamics. To avoid dealing with extremely small time-steps, the Crank-Nicholson unsteady implicit formulation of the above set of equations is used:

\[
R_{u}^{n+1} = \Omega_{CV} \frac{U^{n+1} - U^{n}}{\Delta t} + \frac{1}{2} \left[ R_{s} (V^{n+1}) + R_{s} (V^{n}) \right] = 0 \quad (3.37)
\]

where \( V \) is the vector of primitive variables \((\rho_s, u, v, w, T, k, \omega)\) (note that the form of primitive variable vector used here is different compared to the one used in §3.3). This system is then solved using a sub-iteration procedure to eventually converge to the \((n + 1)^{th}\) time level. For the sub-iteration procedure, the above system can be rewritten as:

\[
R_{u}^{n+1,k+1} = \Omega_{CV} \frac{U^{n+1,k+1} - U^{n}}{\Delta t} + \frac{1}{2} \left[ R_{s} (V^{n+1,k+1}) + R_{s} (V^{n}) \right] = 0 \quad (3.38)
\]

Here each vector to be evaluated at the \((n + 1, k + 1)\) sub-iteration is linearized according to:

\[
R_{s} (V^{n+1,k+1}) = R_{s} (V^{n+1,k}) + \left( \frac{\partial R_{s}}{\partial V} \right)^{n+1,k} \Delta V^{n+1,k} \quad (3.39)
\]

and

\[
U^{n+1,k+1} = U^{n+1,k} + \left( \frac{\partial U}{\partial V} \right)^{n+1,k} \Delta V^{n+1,k} \quad (3.40)
\]

where

\[
\Delta V^{n+1,k} = V^{n+1,k+1} - V^{n+1,k} \quad (3.41)
\]

This linearization and rearrangement of terms will result in the following form of the
discretized equations:

\[
\left[ \frac{\Omega_{CV}}{\Delta t} \frac{\partial U}{\partial V} - \frac{\Omega_{CV}}{2} \frac{\partial S}{\partial V} + \frac{A}{2} \right]^{(n)}_{i,j,k} \Delta V_{i,j,k}^{n+1,k} + \frac{B}{2} \Delta V_{i+1,j,k}^{n+1,k} + \frac{C}{2} \Delta V_{i-1,j,k}^{n+1,k} 
+ \frac{D}{2} \Delta V_{i,j,k+1}^{n+1,k} + \frac{E}{2} \Delta V_{i,j-1,k}^{n+1,k} 
+ \frac{F}{2} \Delta V_{i,j,k+1}^{n+1,k} + \frac{G}{2} \Delta V_{i,j,k-1}^{n+1,k} = -R_u^{n+1,k} \tag{3.42}
\]

Details regarding the evaluation of the flux Jacobians \( \tilde{A} \) through \( \tilde{G} \) can be found in [76]. The above set of equations can be expressed in the form of \( Ax = b \), where \( A \) is a heptadiagonal matrix, \( x = \Delta V^{n+1,k} \), and \( b \) is the residual vector. The correction vector is then solved for using ILU decomposition, and the flow solution is then updated as shown below:

\[
V^{n+1,k+1} = V^{n+1,k} + \Delta V^{n+1,k} \quad \text{and} \quad V^{n+1} = V^{n+1,nmax} \tag{3.43}
\]

where \( kmax \) is the maximum number of sub-iterations per time step.

### 3.4.2 PaSR(1) Equations

The vector form of the equations governing fine-scale properties in the PaSR(1) model can be written as:

\[
R_s = 0 \tag{3.44}
\]

where

\[
R_s = \begin{bmatrix}
P_{1,s,-}^1 - P_{1,s}^2 \\
\vdots \\
P_{NS,s,-}^1 - P_{NS,s}^2 \\
T_s^1 - T_s^2
\end{bmatrix} \tag{3.45}
\]

where

\[
P_{s,s} = (1 - \gamma^*) \left( \frac{\partial (\rho_s^*)}{\partial t} + \frac{1}{\Omega^*} \int_A \rho_s^* \gamma_s^* u_j \cdot n_j dA \right) \tag{3.46}
\]

\[
P_{s,s}^2 = \frac{1}{t_m} (\bar{\rho}_s - \rho_s^*) + (1 - \gamma^*) \tilde{\omega}_s (\rho_s^*, T^*) \tag{3.47}
\]
\[
T_1^* = (1 - \gamma^*) \left( \frac{\partial}{\partial t} \left( \sum_s \rho_s^* h_s(T^*) \right) + \frac{1}{\Omega^*} \int_A \sum_s \rho_s^* h_s(T^*) \gamma^* u_j n_j dA \right)
\]

\[
T_2^* = 1 \cdot \frac{\bar{p} S c \bar{C}_{P,mix} (\bar{T} - T^*)}{\overline{t_m}} + \frac{1}{t_m} \sum_s h_s(\bar{T}) (\bar{p}_s - \rho_s^*)
\]

(3.48)

To achieve time-accuracy, the discretized form of the above set of equations is solved using a sub-iteration procedure, similar to the one used to solve the discretized LES or RANS equations:

\[
R_{n+1,k+1}^* = R_{n+1,k}^* + \left[ \frac{\partial R_s^*}{\partial Q_s^*} \right]^{n+1,k} (\Delta Q_s^*)^{n+1,k} + \left[ \frac{\partial R_s^*}{\partial Q} \right]^{n+1,k} (\Delta Q)^{n+1,k} = 0
\]

(3.50)

where \( Q^* = [\rho_1^*, .., \rho_{NS}^*, T^*] \) is the vector of fine-scale properties and \( Q^* = [\overline{p}_1, .., \overline{p}_{NS}, \bar{T}] \). The terms \((\Delta Q_s^*)^{n+1,k}\) and \((\Delta Q)^{n+1,k}\) are defined as:

\[
(\Delta Q_s^*)^{n+1,k} = (Q_s^*)^{n+1,k+1} - (Q_s^*)^{n+1,k}
\]

\[
(\Delta Q)^{n+1,k} = (Q)^{n+1,k+1} - (Q)^{n+1,k}
\]

(3.51)

Finally, Equation 3.50 can be expressed as:

\[
\left[ \frac{\partial R_s^*}{\partial Q_s^*} \right]^{n+1,k} (\Delta Q_s^*)^{n+1,k} = -R_{n+1,k}^* - \left[ \frac{\partial R_s^*}{\partial Q} \right]^{n+1,k} (\Delta Q)^{n+1,k}
\]

(3.52)

which is in the form of \( Ax = b \), where \( A = \left[ \frac{\partial R_s^*}{\partial Q_s^*} \right]^{n+1,k} \), \( x = (\Delta Q_s^*)^{n+1,k} \), and \( b = -R_{n+1,k}^* - \left[ \frac{\partial R_s^*}{\partial Q} \right]^{n+1,k} (\Delta Q)^{n+1,k} \). The correction vector \( x = (\Delta Q_s^*)^{n+1,k} \) is solved for using ILU decomposition.

### 3.5 Synthetic Eddy Method for Artificial Turbulence Generation

Various methods [81, 65, 82, 83] have been used to generate turbulent inflow conditions for LES, Direct Numerical Simulation (DNS), and LES/RANS. In the present study, one such method, the synthetic eddy method (SEM) of Jarrin et al. [65], is used to generate turbulence in the wall boundary layers and the fuel jets. In this method, instantaneous
velocity fluctuations are generated using input reference statistics, which are available from RANS calculations or DNS. The instantaneous velocity fluctuations \( u'_i \) are calculated using the Cholesky decomposition \( \{a_{ij}\} \) of the Reynolds stress tensor \( R_{ij} \) and a randomized velocity fluctuation field \( \tilde{u}_j \) as shown in Equation 3.53.

\[
u'_i = a_{ij}\tilde{u}_j \tag{3.53}
\]

The Cholesky decomposition \( a_{ij} \) and the randomized velocity fluctuation field \( \tilde{u}_j \) are calculated as shown in Equations 3.54 and 3.55 respectively.

\[
[a_{ij}] = \begin{bmatrix}
\sqrt{R_{11}} & 0 & 0 \\
R_{21}/a_{11} & \sqrt{R_{22} - a_{21}^2} & 0 \\
R_{31}/a_{11} & (R_{32} - a_{21}a_{31})/a_{22} & \sqrt{R_{22} - a_{21}^2 - a_{31}^2}
\end{bmatrix} \tag{3.54}
\]

\[
\tilde{u}_j = \frac{1}{\sqrt{N}} \sum_{k=1}^N \varepsilon_j^k f_{\sigma_{ij}(x)}(x - x^k) \tag{3.55}
\]

where \( k \) indicates the \( k^{th} \) eddy out of a collection of \( N \) eddies located at random locations \( (X^k) \) within a bounding box which spans across the inflow plane where the velocity fluctuations are to be introduced. \( \varepsilon_j^k \) is the intensity of the \( j^{th} \) component of the \( k^{th} \) eddy. Each of these intensities is randomly assigned a value of +1 or -1. The Reynolds stress tensor \( R_{ij} \) is calculated using the input reference statistics. \( f_{\sigma_{ij}(x)}(x - x^k) \), which is defined in Equation 3.56, is the shape function which describes the velocity fluctuation distribution due to the \( k^{th} \) eddy.

\[
f_{\sigma_{ij}(x)}(x - x^k) = \sqrt{V_B} \prod_{j=1}^3 \frac{1}{\sqrt{\sigma_{ij}}} f \left( \frac{x_j - x^k_j}{\sigma_{ij}} \right) \tag{3.56}
\]

where \( \sigma_{ij} \) is the characteristic length scale for the velocity component \( u_i \) in the \( j^{th} \) direction and \( V_B \) is the volume of the bounding box. \( f(x) \), used in calculating the shape function, is defined as shown in Equation 3.57.

\[
f(x) = \begin{cases} 
\sqrt{1.5}(1 - |x|), & \text{if } |x| < 1 \\
0, & \text{otherwise}
\end{cases} \tag{3.57}
\]

After each time step, the new location of each eddy is calculated. This is done by
interpolating the velocity for a particular eddy location using the reference velocity field. If the new eddy location is out of the bounds of the bounding box, then the eddy is replaced with a new eddy, whose location is randomly generated within the bounds of the bounding box. The number of eddies \( N \) randomly distributed within the bounding box is calculated as shown in Equation 3.58.

\[
N = \frac{V_B}{\sigma_{max}^3} \tag{3.58}
\]

where \( \sigma_{max} \) is the largest length scale. The whole process of interpolation and eddy tracking is straightforward for a serial code. The implementation is slightly more complicated in a parallel code, as the entire bounding box can span over multiple blocks that are distributed among multiple processors. In this case, it is not necessary that all eddies be located on a particular processor, as it may not contain the reference data spanning over the entire bounding box. This means multiple data transfers between processors. If the number of processors among which the blocks containing the SEM surfaces are distributed is minimized, then the number of data transfers can be kept to a minimum.

In terms of computational time, this process of eddy tracking and velocity interpolation is the bottleneck in the current implementation of SEM. It is possible to implement SEM by avoiding the tracking and interpolation process. All eddies can be assigned a velocity equal to the nominal freestream velocity. However, this negligence will not accurately represent the reference velocity field. For example, an eddy located inside the boundary layer and close to the wall, will have a velocity that is nearly to zero (or much lower than the freestream velocity). As a result, this eddy will reside inside the bounding box for much longer time than an eddy far away from the wall. These longer residence times mean a more continuous presence of eddies near the walls, which means the shape function for cells close to the walls will be non-zero for longer durations. This ensures that fluctuations generated using the SEM are introduced more regularly near the walls.

The implementations of SEM for wall boundary layers and the fuel jets differ in the way the length scales, reference velocity fields, and Reynolds stresses are calculated. The implementations also differ in the way the bounding boxes are defined, and are described below.

**Wall boundary layers:** A steady-state RANS solution is used for the reference velocity and to calculate the reference Reynolds stresses:
\[ R_{ij} = \frac{\mu}{\rho} \left[ 2 \frac{\partial \tilde{u}_i}{\partial x_i} - 2 \left( \sum_j \frac{\partial \tilde{u}_j}{\partial x_j} \right) \right] + \frac{2}{3} k \]  

(3.59)

\[ R_{ij} = \frac{\mu}{\rho} \left[ \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right] \]  

(3.60)

Instead of using a non-isotropic length scale tensor \((\sigma_{ij})\), which will help in generating non-isotropic turbulent structures close to the walls, a length scale vector \((\sigma_j)\) is used, meaning that the assumption \(\sigma_{1j} = \sigma_{2j} = \sigma_{3j}\) is made. \(\sigma_j\) is calculated as shown in Equation 3.61.

\[ \sigma_j = \max (l, \Delta_j), l = C_\mu \delta \tanh \left[ \frac{\kappa y_d}{C_\mu \delta} \right] \]  

(3.61)

where \(\Delta_j\) is the grid spacing in the \(j^{th}\) direction, \(C_\mu = 0.09\), \(\delta\) is the boundary layer thickness, \(\kappa = 0.41\), and \(y_d\) is the distance from the wall. The bounding box spans over the entire width of the combustor grid. When applied to generate turbulence in the flameholder boundary layers, in the direction perpendicular to the boundary layer, the height of the bounding box is large enough to contain the entire boundary layer well within its bounds. In the case of the boundary layers at the inflow plane of the combustor, the bounding box spans over the entire extent of the inflow plane. Velocity interpolations are determined as follows: First, each eddy is located between the eight adjacent nodes forming a cell in the reference grid. The velocity at this particular location is interpolated between these eight nodes using either tri-linear or inverse distance methods, depending upon the skewness of the cell.

**Hydrogen jets:** DNS databases for pipe flow [84] at two different Reynolds numbers (5300 and 44000) are used to calculate the reference velocity field and Reynolds stresses. Given the injection velocity (1200 m/s) and the diameter of the hole (1 mm), the Reynolds number is 11765. The required reference values are then interpolated for the current Reynolds number (11765) using the \(Re = 5300\) and \(Re = 44000\) databases. An isotropic length scale tensor is used; in other words, it is assumed that \(\sigma_{ij} = \sigma\). The length scale is then calculated as shown in Equation 3.62.

\[ \sigma = \max (\min (l_1, l_2), \max (\Delta_j)), l_1 = \kappa r_d \left( 1 - \exp \left( \frac{-r^+}{26} \right) \right), l_2 = C_2 D \]  

(3.62)
where $r_d$ is the radial distance from the pipe’s wall surface, $r^+ = \frac{u_r r_d}{\nu}$ is the non-dimensional radial wall distance, $C_2 = 0.07$, and $D$ is the pipe diameter. Due to the coarseness of the grid representing the surface of the hole, the grid spacing is always chosen as the length scale. The bounding box is in the shape of a cylinder, which covers the entire hole surface and has a width of the order of the largest length scale. As the properties vary only in the radial direction, calculating the eddy velocities involves one-dimensional interpolation using the reference grid and the reference velocity field.

### 3.5.1 Reference Turbulent Kinetic Energy Matching

It is intuitive that the average turbulent kinetic energy of the fluctuations being introduced using SEM should match with the turbulent kinetic energy of the reference field from the RANS solution ($k_{\text{RANS}}$). To verify this, statistics of SEM generated velocity fluctuations are collected for four combustor-transit-times §6.3.2. Using these statistics, the average turbulent kinetic energy introduced using SEM ($k_{\text{SEM,avg}}$) is calculated. Variations in $k_{\text{RANS}}$ and $k_{\text{SEM,avg}}$, perpendicular to the four walls at the isolator entrance of the Configuration E of UVa’s SCF §4.2.2, along four different lines shown in Figure 3.1, are shown in Figure 3.2. These variations show that, close to the wall, in terms of peak values, $k_{\text{SEM,avg}}$ is half of $k_{\text{RANS}}$, and in general, $k_{\text{SEM,avg}}$ is lower than $k_{\text{RANS}}$. To rectify this, a statistics based correction to $k_{\text{SEM,avg}}$ is implemented. First, the average turbulent kinetic energy introduced using SEM is calculated. This is done by collecting fluctuation statistics for the first 1000 iterations:

$$k_{\text{SEM,avg}} = \frac{1}{1000} \sum_{it=1}^{1000} \frac{1}{2} \left[ (u_1')^2 + (u_2')^2 + (u_3')^2 \right]$$

(3.63)

After the values of $k_{\text{SEM,avg}}$ stabilize (for iterations $it > 1000$), the fluctuations introduced using SEM are scaled using the ratio $k_{\text{RANS}}/k_{\text{SEM,avg}}$:

$$u_{i,\text{Scaled}} = \sqrt{\frac{k_{\text{RANS}}}{k_{\text{SEM,avg}}}} u_i'$$

(3.64)

As shown in Figure 3.2, this statistics based correction helps in matching the average turbulent kinetic energy introduced through SEM with the reference turbulence kinetic energy from the RANS solution.
Figure 3.1: Lines perpendicular to the four walls at the inflow plane of Configuration E of UVa’s SCF (see §4.2.2), along which variation of $k$ is plotted.
Figure 3.2: Variations of $k_{RANS}$, $k_{SEM,avg}$, and $k_{SEM,scaled}$ perpendicular to the four walls at the inflow plane of Configuration E of UVa’s SCF (see §4.2.2)
Chapter 4

Scramjet Experiments

4.1 DLR Scramjet Experiment

The DLR scramjet combustor facility is comprised of two basic parts: a Laval nozzle through which preheated air is expanded, and a combustor into which the preheated air enters and where the actual combustion process takes place. A schematic of the facility is shown in Figure 4.1. The combustor has a height of 5 cm and an upper wall with a diverging angle of 3 degrees. A wedge shaped injector, with a half angle of 6 degrees, is placed at the center of the combustor. The wedge is 32 mm long, and the base of the wedge is 6 mm wide. Hydrogen is injected at sonic conditions through fifteen holes with a diameter of 1 mm, located on the base of the wedge. The distance between the centers of adjacent holes is 2.4 mm. The dimensions of the combustor are shown in Figure 4.2, and the nominal freestream conditions used in all the calculations are shown in Table 4.2.

To qualitatively compare the results from all the simulations performed in the present work, predicted profiles are presented at eight different stations. However, experimental data is not available at all eight stations. The locations of these eight stations and the availability of experimental data at each of these stations are shown in Table 4.1. Experimental data is available in the form of: axial velocity profiles (measured using Laser Doppler Velocimetry (LDV)) at Stations 1, 4, and 7 for reactive flow and at Stations 1, 4, 5, and 8 for non-reactive flow; static temperature profiles (measured using Coherent Anti-Stokes Raman Spectroscopy (CARS)) at Stations 1, 4, and 8 for reactive flow; and axial velocity fluctuation profiles (measured using LDV) at Stations 1, 4, and 5 for reactive flow and at Stations 6 and 7 for non-reactive flow. Axial velocity values along the geometric
centerline of the combustor (measured using LDV) for reactive and non-reactive flows, static pressure measurements along the geometric centerline for non-reactive flow, and static pressure measurements along the lower wall for reactive and non-reactive flows are also available from experiments.

Figure 4.1: Schematic overview of the DLR scramjet combustor facility (images from Waidmann et al. [8])
Figure 4.2: Dimensions of the DLR scramjet combustor

Table 4.1: DLR combustor: Available experimental data at various stations (station locations indicated in meters; “R” and “NR” mean Reacting and Non-Reacting flows, respectively)

<table>
<thead>
<tr>
<th>Data type</th>
<th>Station 1</th>
<th>Station 2</th>
<th>Station 3</th>
<th>Station 4</th>
<th>Station 5</th>
<th>Station 6</th>
<th>Station 7</th>
<th>Station 8</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$x = 0.120$</td>
<td>$x = 0.132$</td>
<td>$x = 0.141$</td>
<td>$x = 0.167$</td>
<td>$x = 0.199$</td>
<td>$x = 0.224$</td>
<td>$x = 0.249$</td>
<td>$x = 0.275$</td>
</tr>
<tr>
<td>Axial velocity</td>
<td>R</td>
<td>NR</td>
<td>R</td>
<td>NR</td>
<td>R</td>
<td>NR</td>
<td>R</td>
<td>NR</td>
</tr>
<tr>
<td>Static temperature</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Axial velocity fluctuations</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
</tbody>
</table>
Table 4.2: DLR combustor: Inflow conditions for incoming air and hydrogen jets

<table>
<thead>
<tr>
<th>Property</th>
<th>freestream</th>
<th>Injector holes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_\infty \ (\frac{m}{s})$</td>
<td>730.0</td>
<td>1200.0</td>
</tr>
<tr>
<td>$T_\infty \ (K)$</td>
<td>340.0</td>
<td>250.0</td>
</tr>
<tr>
<td>$P_\infty \ (\text{bar})$</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$Y_{N_2}$</td>
<td>0.736</td>
<td>0.0</td>
</tr>
<tr>
<td>$Y_{O_2}$</td>
<td>0.232</td>
<td>0.0</td>
</tr>
<tr>
<td>$Y_{H_2}$</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$Y_{H_2O}$</td>
<td>0.032</td>
<td>0.0</td>
</tr>
</tbody>
</table>
4.2 University of Virginia’s Scramjet Combustion Facility

The University of Virginia’s Scramjet Combustion Facility (UVa’s SCF) is a dual-mode ramjet/scramjet combustor capable of simulating flight conditions at Mach 5 enthalpy. It consists of a Mach 2 inlet nozzle, a constant-area isolator, a combustor, and an extender, through which the exhaust gases are vented to the atmosphere. A schematic overview of the facility is shown in Figure 4.3. For more details regarding UVa’s SCF, the reader is referred to Fulton et al. [28].

Figure 4.3: Schematic overview of the UVa’s SCF [9]
4.2.1 Configuration A

Experiments have been performed on different configurations of the actual facility. In Configuration A of the UVa’ SCF, the Mach 2 nozzle is directly connected to the combustor section (no isolator). Hydrogen is injected through a converging-diverging nozzle located on the leeward side of a single, unswept, three-dimensional compression ramp, the base of which is located on the upper wall of the combustor section. The angle between the upper ramp surface and the upper wall of the combustor is 10°, and the height of the base of the ramp (H) is 0.25 inches (6.35 mm). Hydrogen is injected in a direction parallel to the upper ramp surface at an approximate Mach number of 1.7.

Detailed dimensions of this configuration are shown in Figure 4.4. The nominal freestream and stagnation values used in the experiments are shown in Table 4.3. Experimental measurements include CARS measurements of mean and \textit{rms} temperatures, \textit{O}_2 mole fraction, \textit{N}_2 mole fraction, and \textit{H}_2 mole fraction at three stations (x/H = 6, 12, and 18) \[85\]; stereoscopic PIV measurements at one station (x/H = 12) \[86, 87, 88\]; \textit{OH}-PLIF images at several stations between x/H = 0 and x/H = 12 \[89\]; and centerline wall pressure distributions. Here, a station indicated as x/H = C means that the station is located at x = H×C inches downstream of the ramp base. Configuration A of UVa’s SCF shall be addressed from here on as the UVa-A combustor.

Table 4.3: Configuration A of UVa’s SCF: Mean freestream and stagnation values used in the Mach 2 nozzle, injector nozzle, and combustor simulations

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach 2 nozzle stagnation pressure</td>
<td>295.0 kPa</td>
</tr>
<tr>
<td>Mach 2 nozzle stagnation temperature</td>
<td>1200 K</td>
</tr>
<tr>
<td>Mean combustor inflow pressure</td>
<td>38000.0 Pa</td>
</tr>
<tr>
<td>Mean combustor inflow temperature</td>
<td>667.0 K</td>
</tr>
<tr>
<td>Mean combustor inflow velocity</td>
<td>1035.0 m/s</td>
</tr>
<tr>
<td>Hydrogen stagnation pressure</td>
<td>458410.0 Pa</td>
</tr>
<tr>
<td>Hydrogen stagnation temperature</td>
<td>298.0 K</td>
</tr>
<tr>
<td>Equivalence ratio</td>
<td>0.17</td>
</tr>
</tbody>
</table>
Figure 4.4: Dimensions of Configuration A of University of Virginia’s dual-mode scramjet [9] (side-view: top image and top-view: bottom image). All dimensions are normalized using the compression ramp height (H) of 0.25 inches.
4.2.2 Configuration E

In Configuration E, ethylene is used as fuel instead of hydrogen. To increase the fuel-residence time, Configuration E is fitted with a cavity on the upper wall of the combustor section. Also, the three-dimensional ramp injector is removed, and ethylene can be injected through a series of ports (three rows of ports upstream of the cavity and one row of ports inside the cavity, with each row consisting of five fuel-injecting ports) located along the upper wall of the combustor section. For the case considered in the present study, ethylene is injected through the most upstream row of injectors. The locations of these injection ports and the overall design of Configuration E are shown in Figure 4.6. Unlike Configuration A, Configuration E has the isolator and an additional constant area extender in place.

The inflow conditions for air are the same as in Configuration A. To achieve an equivalence ratio of 0.15 (mass flow rates of ethylene and air are 1.87 gm/s and 182.75 gm/s, respectively), ethylene is injected at the following stagnation conditions: 973296.3 Pa and 298.0 K. For this equivalence ratio, experimental data is available in the form of Line-of-Sight (LOS) measurements of species mole-fractions, column-densities, and temperatures, which are measured using Tunable Diode Laser Absorption Spectroscopy (TDLAS) at three different stations [90]. The locations of these stations are shown in Figure 4.5, and the available experimental data at each of these stations is shown in Table 4.4. Also, pressure measurements along the upper wall of the combustor are available from experiments. Configuration E of UVa’s SCF shall be addressed from here on as the UVa-E combustor.

Table 4.4: Configuration E of UVa’s SCF: Experimental data available through TDLAS measurements; CD: Column-density, T: temperature, and X: mole-fraction

<table>
<thead>
<tr>
<th>Station</th>
<th>CD$_{H_2O}$</th>
<th>T$_{H_2O}$</th>
<th>CD$_{CO}$</th>
<th>T$_{CO}$</th>
<th>CD$_{CO_2}$</th>
<th>X$_{H_2O}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>2</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>3</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
</tr>
</tbody>
</table>
Figure 4.5: Configuration E of UVa’s SCF: Location of the stations at which experimental data is available (all dimensions in inches)
(a) Side-view

(b) Zoomed in view of the combustor section

Figure 4.6: Dimensions of Configuration E of UVa’s SCF (diameter of the injection ports is 0.021 inches; all dimensions in inches)
Figure 4.7: Zoomed in view of the cavity section of Configuration E of UVa’s SCF (all dimensions in inches)

\textbf{Computation of LOS Data}

Column-density of species $s$ is defined as the path-integral of number-density (molecules per unit volume) along the LOS:

\[ \text{CD}_s = \int_0^L n_s \text{d}l = \int_0^L \frac{\rho_s}{M_s} N_A \text{d}l \]  

(4.1)

where $N_A$ is the Avagadro constant. Temperature of species $s$ is the number-density-weighted average temperature:

\[ T_s = \frac{\int_0^L n_s T \text{d}l}{\int_0^L n_s \text{d}l} = \frac{\int_0^L n_s T \text{d}l}{\text{CD}_s} \]

(4.2)
For the coordinate system used in the grid representing the UVa-E combustor, the lines-of-sight, along which the path-integrals are to be calculated, extend in the z-direction (lines with constant x- and y-coordinates). The predicted line-of-sight data is calculated by first extracting the instantaneous flow solution over a rectangular array of points spread across a particular cross-plane, the location of which coincides with one of the stations where experimental data is available. Then, the path-integrals are calculated by numerically integrating the data extracted along these lines-of-sight.

4.3 Facility-Dependent Effects

4.3.1 DLR Combustor: Non-Uniform Inflow Generation

For the DLR combustor, preheated air is first expanded through a Laval nozzle, which is attached to the inlet of the combustor. This means that a boundary layer and shock system develop inside the Laval nozzle and then propagate into the combustor. To account for these, flow through the Laval nozzle is first simulated using RANS techniques. As there is no detailed description of the nozzle design available, the nozzle shape was digitized from the scramjet-facility image provided in Waidmann et al. [8] (Figure 4.1a). Using the digitized shape of the nozzle, a structured multi-block grid is generated, which is shown in Figure 4.8. The nozzle grid and the combustor grid have a set of common blocks, which are used to impose the nozzle exit conditions as inflow conditions for the combustor.

Based on the freestream conditions specified in Waidmann et al. [35, 36, 8] for the combustor inflow, stagnation conditions are calculated using isentropic flow equations. These stagnation conditions are then used to specify the inflow conditions for the Laval nozzle. In Figure 4.9, centerplane density-gradient contours for the flow through the Laval nozzle are shown, which clearly show the boundary layers along the walls and the shock structure inside the Laval nozzle. The inflow boundary condition for the DLR combustor obtained from this RANS simulation is referred to from here on as the non-uniform inflow, which is used in a number of simulations discussed in the present work. This non-uniform inflow plays a very crucial role in the prediction of the flame structure, which will be discussed in §5.2.
Figure 4.8: Structured multi-block grid for the Laval nozzle attached to the DLR combustor

Figure 4.9: Density-gradient contours inside the DLR Laval nozzle
4.3.2 UVa’s SCF: Thermal Non-Equilibrium and Non-Uniform Inflow

The CARS measurements reported in [91] showed that the air entering the isolator section of UVa’s SCF, after passing through the Mach 2.0 nozzle, was in a state of thermal non-equilibrium. Specifically, the vibrational temperatures of nitrogen and oxygen were observed to be 1200 and 1000 K, respectively; rotational and translational temperatures of nitrogen and oxygen relaxed to around 735 K. Currently, NCSU’s REACTMB is not equipped to handle thermal non-equilibrium. To account for the thermal non-equilibrium effects in a thermally-equilibrated sense, at each CARS measurement point, the specific internal energies of the equilibrium and non-equilibrium states are matched with each other to obtain the effective equilibrium temperature. More details about this procedure can be found in [9].

Also, the same CARS measurements revealed that the various temperature distributions were not uniform across the isolator inflow cross-section. This non-uniformity is accommodated into the simulations by first calculating the effective equilibrium temperatures using the procedure described above. These effective equilibrium temperatures were then used to calculate the non-uniform stagnation temperatures:

\[
\sum_k Y_k (h_k(T_0) - h_k(T_{eq})) = \frac{1}{2} |\bar{V}|^2
\] (4.3)

These non-uniform stagnation temperatures were the used for specifying the inflow boundary condition for the Mach 2 nozzle. Values for velocities (\(\bar{V}\) in Equation 4.3) at each of the CARS points were obtained from the simulations performed assuming uniform temperature distributions. Again, more details regarding the implementation of this procedure can be found in [9]. The non-uniform temperature profile at the entrance of the isolator is shown in Figure 4.10.
Figure 4.10: Cross-plane contours of temperature at the entrance of the isolator for UVa’s SCF
Chapter 5

Effect of Algorithmic and Modeling Choices

5.1 DLR Combustor in its Entirety

In this section, results are presented from the first attempts made at simulating the non-reactive and reactive flows through the DLR combustor. Both RANS and LES/RANS techniques are used on a grid where the combustor in its entirety is considered (all fifteen fuel-injecting holes and side walls). Results from these simulations and various issues faced are presented and discussed in the current section.

5.1.1 Grid

First, separate multi-block structured meshes are used to represent the Laval nozzle and the combustor in the computational domain. The combustor mesh, shown in Figure 5.1, is comprised of 2085 blocks and 33,141,428 interior mesh cells. The average mesh spacing in the mixing region is $5 \times 10^{-4}$ m, and the minimum mesh spacing at all solid surfaces is $5 \times 10^{-6}$ m.

5.1.2 Initial and Boundary Conditions

Initially, RANS equations are solved to simulate the non-reactive flow through the combustor; this simulation is initialized by specifying the freestream values throughout the combustor domain. Steady state solution from this simulation is then used to initialize
Figure 5.1: DLR combustor: Multi-block structured mesh
the RANS reactive and LES/RANS non-reactive simulations. In the RANS reactive simulation, the fuel is ignited by lowering the activation energies in the region close to the backplane of the injector. Then, steady state solution from the RANS reactive run is used to initialize the LES/RANS reactive simulation.

As stated in §4.3.1, the flow through the Laval nozzle is first computed by solving the RANS equations, and the conditions obtained at the exit plane of the nozzle are used as the inflow conditions for the combustor calculations. Following the works of Berglund & Fureby [34] and Genin & Menon [92], all walls are treated as adiabatic, non-slip boundaries. Since the reacting zones are far away from the upper and lower walls, the direct influence of the adiabatic upper and lower walls on the flame is negligible. However, this assumption can have an influence on the boundary layer growth and shock structure, which have a direct influence on the flame structure. Since these experimental details are not available, and based on the quality of results from the works of Berglund & Fureby [34] and Genin & Menon [92], this assumption is considered reasonable. The adiabatic side walls can have a direct influence on the flame. None of the previous works that simulated the flow through the DLR combustor considered side walls in their computational domain. So, regarding the side walls, not much information is available either from experiments or from previous works. At the exit plane of the combustor, the fluid properties are extrapolated from the interior cells. The round topology of the fuel-injecting holes is not rendered. Instead, a blanking function is used to distinguish between regions that are to be treated as walls or supersonic inlets.

5.1.3 Time Advancement

In RANS simulations, the desired end result is to reach a steady state solution at a high rate of convergence. To this end, in RANS simulations, a local time step is used for each computational cell. In LES, spatially averaged instantaneous Navier-Stokes equations are solved; so after each temporal iteration, it is essential that the solution is time-accurate. To achieve this, the LES/RANS solutions are evolved at a global (same time step for all cells) constant time step of $1.5 \times 10^{-7}$ seconds using the sub-iteration procedure described in §3.4.1.

The time required for a fluid element traveling at 730 m/s to traverse the average mesh spacing in the mixing region ($5 \times 10^{-4}$ m) is $6.849 \times 10^{-7}$ seconds. This and the constant time step chosen result in a Courant-Friedrichs-Lewy value of 0.219, which is small enough
to ensure good convergence of the sub-iterations. First, the LES/RANS simulations are evolved for two flow-through-times to eliminate initial transients associated with the RANS base state. One flow-through-time is defined as the time required for the flow at the nominal freestream velocity to travel from the wedge base to the combustor exit. Distance between the wedge base and the combustor exit plane is 0.231 m, and the freestream velocity is 730.0 m/s, which means one flow-through-time is approximately 0.0003164 seconds. Time averages are then collected for upwards of four flow-through-times times. Unless otherwise noted, the results presented later are obtained by span-averaging the time-averaged data over a length equal to the distance between three injector holes and spanning the z-centerline of the combustor.

### 5.1.4 Results

Results are presented for cases with and without combustion. Instantaneous centerplane temperature contours of the reactive flow are shown in Figure 5.2, which illustrate the general predicted flame structure. In the DLR combustor, the mixing process is dominated by large, Kelvin-Helmholtz-type roller structures that originate at the trailing edges of the flameholder; in this way the flame structure is more two-dimensional than three-dimensional. The roller structures collect pockets of air from the freestream, which are then entrained into the flame front, increasing the heat transfer away from the front. The predicted flame is detached in all simulations; however, the flame periodically moves upstream towards the base of the flameholder.

The instantaneous contours of density gradient for the non-reactive and reactive cases are shown in Figures 5.3a and 5.3b, respectively. At the inflow plane of the combustor, two shocks originating inside the Laval nozzle enter the combustor and reflect off the wedge surface. Two strong shocks originate from the leading edge of the wedge. These four shocks reflect off the walls of the combustor multiple times and interact with each other at various points. At the two corners of the wedge, expansion fans are produced, both of which impact the upper and lower walls. It is evident that the expansion fans span over a larger area for the non-reactive case, compared with the reactive case. For the non-reactive case, further downstream, the expanding flow re-compresses through a series of weak shocks. These shocks coalesce to form a strong shock which impacts the upper wall, creating a separation bubble. The displacement effect of this separation bubble results in the formation of a shock, an expansion fan, and a reattachment shock,
Figure 5.2: DLR combustor: Instantaneous temperature contours for the reactive flow all three of which are clearly visible in Figure 5.3a.

Figure 5.3: DLR combustor: Shock structures predicted for the non-reactive and reactive flows
The shock structures shown in Figures 5.3a and 5.3b are from simulations where the zonal hybrid LES/RANS model, described in §2.2.5, is used. To justify the usage of the zonal hybrid LES/RANS model, a closer view of the shock structure inside the combustor for the non-reactive flow, when the LES/RANS method of Gieseking et al. [69] is used for the wall boundary layers without inflow forcing, is shown in Figure 5.4a. In this case, the sizes of the initial separation bubbles, produced on the upper and lower walls of the combustor due to the impingement of the leading edge shocks, are too large. The resulting complicated system of shocks and expansion waves is a clear deviation from the shock structure observed in the experiments, which is shown in Figure 5.4c. Using the zonal hybrid LES/RANS model leads to a better response for this case (Figure 5.4b).

It is important to mention that the non-uniform inflow boundary is used in both simulations (Figures 5.4a and 5.4b). Because of the non-uniform inflow, three distinct shocks entering the combustor from the nozzle reflect off the injector surfaces and impinge on the upper and lower walls at the center of Figure 5.4b. The second of these three shocks is the strong shock that is formed due to the combination of two weaker shocks entering the combustor because of the non-uniform inflow. The experimental Schlieren image also shows three distinct shocks impinging on the lower wall at the same location. This confirms that the shocks generated by using the non-uniform inflow were also observed in experiments.

In this section, results from the non-reactive and reactive flow simulations are discussed and compared with the experimental data.

**Non-Reactive Flow**

Axial velocity profiles (at various x-locations downstream of the base of the wedge) from RANS and LES/RANS simulations are compared with experiments in Figure 5.5. At Station 1 (x = 0.120 m), in the wake of the wedge, the axial velocity is under-predicted compared to the experiments. At Station 4 (x=0.167 m) and locations further downstream, the RANS predictions are generally in better agreement with experiment than the LES/RANS predictions. The fact that the LES/RANS profiles appear more uniform may mean that the eddy sizes are over-predicted, increasing momentum transfer rates between the freestream and the wake.

In Figure 5.6, axial velocity fluctuation profiles from the LES/RANS simulation are compared with experimental measurements. Good agreement in terms of peak magnitude
(a) Instantaneous density-gradient contours with LES/RANS method of Gieseking et al. [69] used near the walls

(b) Instantaneous density-gradient contours with blending (from Equation 2.86) used near the walls

(c) Experimental shadow graph [92]

Figure 5.4: DLR combustor: Predicted and experimental shock structures for the non-reactive flow
is indicated; however, there seems to be a shift of the peak values in the y-direction. This shift is evident in the axial velocity profiles as well. The experiment also indicates a high level of freestream turbulence, which is not modeled in the simulation. Axial velocity and static pressure distributions along the geometric centerline of the combustor are shown in Figures 5.7a and 5.7b, respectively. In the wake region near the base of the wedge, both RANS and LES/RANS models predict a steep increase and then a decrease of axial velocity, which is a deviation from the experimental measurements. These values correspond to the velocities of the hydrogen jet before the mixing process commences. Both RANS and LES/RANS models provide similar pressure distributions along the geometric center-line. The shocks from the leading edge of the wedge, after reflecting from the upper and lower walls, pass through the wake. As a result, the pressure distributions predicted by RANS and LES/RANS in Figure 5.7b show a rise in the pressure in two successive steps between x=0.14 m and x=0.15 m. This pattern in the pressure rise is in good agreement with the experimental results. However, experimental results show higher pressure values in this region.

The static pressure predictions along the lower wall, shown in Figure 5.7c, are nearly the same for RANS and LES/RANS. This is not surprising given the fact that both RANS and LES/RANS use the same turbulence model inside the boundary layer. The expansion fan originating from the lower edge of the injector comes in contact with the lower wall between x=0.125 m and x=0.175 m. Due to this impact, there is a steady decrease in the pressure along the lower wall in this region. This decrease in pressure, predicted by RANS and LES/RANS, matches well with the experimental measurements. A series of weak shocks, resulting from the interaction of the freestream and the shear layers between x=0.112 m and 0.145 m, combine to form two strong shocks, one of which impacts the lower wall at x=0.175 m. This results in an increase in pressure along the lower wall. Two more shocks, after reflecting from the upper wall, impact the lower wall between x=0.175 m and 0.2 m. The first one is the leading edge shock and the second one is a weak shock that originates in the Laval nozzle. Due to the impact of both the shocks with the lower wall, there is a further increase in pressure in two steps. Experimental results lack the resolution to show conclusively whether the pressure rises in a single step or multiple steps. But the experimental shadow graph, shown in Figure 5.4c, shows that the three shocks impact the lower wall at different points. Again, the experimental measurements show a higher rise in pressure due to the shock impingement compared to the simulation.
results.

Figure 5.5: DLR combustor: Axial velocity profiles for the non-reactive case

Figure 5.6: DLR combustor: Axial velocity fluctuation profiles for the non-reactive case
Figure 5.7: DLR combustor: Axial velocity profiles along the geometric centerline (top) and static pressure profiles along the geometric centerline (middle) and lower wall (bottom) for the non-reactive cases
Reactive Flow

The shock structure for the reactive flow through the DLR combustor is shown in Figure 5.3b. The flame structure is also clearly visible. Because of volumetric expansion of the plume due to heat release, the shock pattern downstream of the wedge’s base is completely different from that of the non-reactive case. The reactive case is simulated using:

1. RANS - 9 Species: RANS equations are solved. The hydrogen oxidation process is modeled using a nine-species, eighteen-step reaction mechanism [2].

2. LES/RANS - 9 Species: Zonal hybrid LES/RANS technique 2.2.5 is used in conjecture with the same nine-species, eighteen-step reaction mechanism used in RANS.

3. LES/RANS - 7 Species: Zonal hybrid LES/RANS technique is used in conjecture with a seven-species, seven-step reaction mechanism [3, 4].

The results from the three cases differ substantially. Time-averaged static temperature contours for the plane passing through the middle of the combustor are shown for all three cases in Figure 5.8. In three cases, the flame is detached from the base of the wedge. The flame is thicker just downstream of the wedge and is hotter throughout for the RANS case compared to the other two cases. The hot zone of the flame for the LES/RANS 9-species case extends for a longer distance in the x-direction and is thicker compared to the LES/RANS 7-species case. Time-averaged contours of OH mass fraction in Figure 5.9 show that the largest amount of OH is produced in the region where the temperature is the highest. Since the LES/RANS methods more directly capture the effects of resolved turbulent eddies in locally straining the flame, the overall entrainment of fluid from the freestream into the flame front is higher in the LES/RANS simulations. This increases the heat transfer away from the flame front and reduces the reactivity of the mixture accordingly. It appears that the seven-step hydrogen-air mechanism is more susceptible to such effects at the mesh scale, as the overall level of heat release is obviously lessened.

Figure 5.10 shows axial-velocity profiles (from predictions and experiment) at three different locations downstream of the wedge. At Station 1 (x=0.120 m), which is the closest station to the wedge, all three predictions do not show a particularly good match with the experimental data. Both 9-species and 7-species LES/RANS predictions show a peak in the velocity profile at y=0.025 m, which is due to the hydrogen jet. A similar peak in the profile can be seen in the experimental data as well, but the velocities in the
Figure 5.8: DLR combustor: Contours of time-averaged temperature
Figure 5.9: DLR combustor: Contours of time-averaged OH mass fraction
core region are higher in the experiment. At Station 4 ($x = 0.167$ m), the peak in the velocity profile is best predicted by the LES/RANS model with 9-species kinetics, but in the freestream region, RANS predictions show better agreement with the experiment. The degree of volumetric expansion of the reacting plume is highest for the RANS model, and as a result, the core flow is compressed more, leading to lower core flow velocities. At Station 7 ($x = 0.249$ m), the variation in the axial velocity among the models is not as high as it is at Stations 1 and 4. Overall, the LES/RANS 7-species prediction agrees best with the experimental profile.

![Axial velocity profiles for the reactive cases](image)

**Figure 5.10: DLR combustor: Axial velocity profiles for the reactive cases**

The axial-velocity fluctuation profiles are shown in Figure 5.11 at Stations 1, 4, and 5. Both 9-species and 7-species LES/RANS predictions agree well with the experimental data in the wake region of the wedge. In the freestream region, there is again an under-prediction of the intensity levels due to the absence of freestream turbulence in the simulations.

Static temperature predictions are compared with experimental data in Figure 5.12. At Station 1 ($x = 0.120$ m), all three cases under-predict the static temperature. This is consistent with the static temperature contours shown in Figure 5.8 in that conditions favorable for significant heat release are not found until the very end of the mixing region. The experiment indicates that the reaction zone is anchored within the recirculation regions downstream of the wedge base. Animations of the numerical flame response indicate that the computed flame alternately attaches and detaches from the top and
bottom trailing edges of the wedge. A modest rise in temperature at Station 1 due to these events is noted in Figure 5.12, but the general trend is for the flame to lift away from the wedge back plane and to be stabilized in a small recirculation region located near the centerline (discussed later). RANS results show an over-prediction of static temperature for Stations 4 and 8. The flame thicknesses and the peak temperatures are best predicted by the LES/RANS model with 7-species kinetics at these stations.

Figure 5.11: DLR combustor: Axial velocity fluctuation profiles for the reactive cases

Figure 5.12: DLR combustor: Static temperature profiles for the reactive cases
Axial velocity predictions along the geometric centerline of the combustor are shown in Figure 5.13a. The results from LES/RANS simulations show a steep decrease in the velocity values from around 1100 m/s to negative values. This region with negative axial-velocities, between $x = 0.125$ m and $x = 0.155$ m, corresponds to a recirculation zone located downstream of the location of maximum penetration of the hydrogen jet array. This recirculation zone is clearly visible in Figure 5.14, where the velocity vectors are shown downstream of the wedge base. While the LES/RANS model predictions are similar between $x = 0.109$ m and $x = 0.200$ m, the LES/RANS 7-species predictions show the best agreement with experiment for $x > 0.200$ m.

The static pressure profiles along the lower wall, shown in Figure 5.13b, are significant in the sense they predict the locations where the shocks reflect from the walls. The predictions from all three cases are same for the region $x < 0.145$ m. However, downstream of this location, the predictions differ substantially. As the flame structure changes, the locations where the shocks reflect and the angles of reflection change. As a result of this, the magnitudes of the pressure increases due to the impact of the shocks on the wall are also different. None of the predictions are in particularly good agreement with experiment though the LES/RANS 7-species results appear to follow the experimental trends most closely.
Figure 5.13: DLR combustor: Axial velocity profiles along the geometric centerline and static pressure profiles along the lower wall for the reactive cases
Figure 5.14: DLR combustor: Velocity vectors showing the recirculation region in the flame
5.2 Spanwise Periodicity

Results discussed in §5.1.4 show that the predicted flame is lifted in all cases. However, experiments suggest that the observed flame is either attached or at the least closer to the base of the injector than the predicted flame. Results from the attempts made to address this issue (to better predict the flame stabilization location) are presented in the current section.

An under-prediction in the fuel-air mixing could have led to inaccuracy in the predicted flame position. Using a finer grid can help in directly resolving more turbulence, which will enhance the fuel-air mixing rate in the simulations. With this idea in mind, in the current section, finer grids capable of capturing higher amounts of turbulence are generated. To keep the computational cost manageable, only five of the fifteen fuel-injecting holes are considered and periodicity is assumed in the spanwise direction. Initial simulations show that the influence of the side walls on the predictions near the centerplane of the combustor is minimal. So, the assumption of periodicity in the spanwise direction is justified to a certain extent. Other modeling and algorithmic choices are also varied in an attempt to improve the overall predictive capability of the solver.

5.2.1 Grid Topologies

The topology around the injector for the grid used in §5.1, where all fifteen fuel injecting holes are considered, is shown in Figure 5.15a. In this grid, the clustering near the injector wall surfaces is wrapped around the body of the injector. This ensures that the grid is isotropic and uniform further downstream. But, this topology is not adequate for resolving the turbulent fluctuations in the shear layers. To address this issue, the grid topology is changed to the one shown in Figure 5.15b; this grid shall be addressed from here on as Grid A. Considering the high velocity gradients at the edge of the hydrogen jets, another grid (Grid B) is generated by clustering the cells at the injector holes’ boundaries, shown in Figure 5.15c. This clustering is evened out gradually downstream of the injector face. Grids A and B are used in all the simulations discussed in the current section.

Grids A and B consist of 12,595,720 and 20,337,300 cells, respectively. The average cell size in the mixing region is $2.5 \times 10^{-4}$ m, which is half of what it is in the grid used in §5.1. The minimum mesh spacing at all solid walls is $5 \times 10^{-6}$ m, except at the back plane of the injector, where the minimum mesh spacing is increased to $2 \times 10^{-5}$ m. Also,
to limit the number of mesh cells, the axial extents of Grids A and B are reduced from \( x=0.340 \) m (grid used in §5.1) to \( x=0.285 \) m.

### 5.2.2 Initial and Boundary Conditions

All simulations performed using Grids A and B are initialized in the same way as the simulations discussed in §5.1. Again, only five of the fifteen fuel-injecting holes are considered, and periodicity is assumed in the spanwise direction. Similar to §5.1, all walls are treated as adiabatic, non-slip boundaries, and the fluid properties are extrapolated from the interior cells at the exit plane of the combustor. Two different inflow conditions, uniform and non-uniform, are used for the inflow boundary of the combustor. As described in §4.3.1, the non-uniform profiles for various variables are obtained by simulating the flow.
through the attached nozzle using RANS techniques, which is the same inflow boundary used in §5.1. For the uniform inflow condition (nominal freestream conditions from Table 4.2 are used), the value of each variable is constant across the entire combustor inflow plane. In other words, the two-dimensional profile of a particular variable, across the inflow plane of the combustor, is uniform. As in §5.1, the round topology of the fuel-injecting holes is not rendered. Instead, a blanking function is used to distinguish between regions that are to be treated as walls or supersonic inlets.

5.2.3 Time Advancement

All LES/RANS calculations are evolved at a constant time-step of $1 \times 10^{-7}$ seconds. The time required for a fluid element traveling at the nominal freestream velocity of 730 m/s to traverse the average mesh spacing in the mixing region (0.25 mm) is $3.42 \times 10^{-7}$ s. The time step chosen for the simulations corresponds to a global Courant-Friedrichs-Lewy value of about 0.3 and is small enough to ensure good convergence of the sub-iterations. To reach a statistically steady state, the flow is allowed to evolve for two flow-through-times. For Grids A and B, distance between the injector base and the combustor exit plane is 0.176 m, and the nominal freestream velocity is 730.0 m/s, which means one flow-through-time is approximately 0.000241 seconds. Time averages are then collected for four flow-through-times. Results presented in the form of line-plots are span-averaged over the entire spanwise length of the Grids A and B, which span across five fuel-injecting holes.

5.2.4 Cases

Several parametric studies are conducted with a view toward improving the overall predictive capability of the solver and determining the sensitivities of the predictions to modeling and algorithmic variations. These variations include grid topologies, flux reconstruction methods, reaction mechanisms, and SEM for aiding mixing. If these variations are viewed as choices, then starting from a baseline case, each choice is changed one at a time to narrow down the effect it has on the simulated flow. Two different grid topologies, Grid A and Grid B, shown in Figures 5.15b and 5.15c respectively, are used. The two grids are different in the sense that Grid B has higher resolution near the hydrogen jets’ boundaries to resolve the high velocity gradients in this region. To model
hydrogen oxidation, two reaction mechanisms (Jachimowski [2] and Ó Connaire [5]) are used. The effects of TVD [78] and PPM [79] reconstruction methods are also investigated. To aid fuel-air mixing, a synthetic eddy method [65] is used to increase the turbulence levels in the shear layers and the hydrogen jets. For most of the initial simulations (Cases 1 through 6), a uniform inflow boundary condition is used. The non-uniform inflow boundary, described in §4.3.1, is used in Case 7. All the cases simulated in the present study are shown in Table 5.1.

Table 5.1: DLR combustor: Modeling choices made in various cases

<table>
<thead>
<tr>
<th>Cases</th>
<th>Grid topology</th>
<th>Reaction mechanism</th>
<th>Reconstruction method</th>
<th>SEM for shear layers</th>
<th>SEM for hydrogen jets</th>
<th>Non-uniform inflow</th>
</tr>
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<tbody>
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<td>TVD</td>
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<td>No</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>Grid A</td>
<td>Ó Connaire</td>
<td>TVD</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>Grid A</td>
<td>Ó Connaire</td>
<td>PPM</td>
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<td>No</td>
<td>No</td>
</tr>
<tr>
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<td>Ó Connaire</td>
<td>PPM</td>
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<td>Yes</td>
<td>No</td>
</tr>
<tr>
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<td>No</td>
</tr>
<tr>
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</tr>
<tr>
<td>7</td>
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<td>Ó Connaire</td>
<td>PPM</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

5.2.5 Results

Non-Uniform vs. Uniform Inflow for Reactive Flow

The instantaneous density-gradient contours for the reactive flow through the combustor, with uniform and non-uniform inflow conditions, are shown in Figure 5.16. Depending
upon the type of inflow boundary used, the shock structure inside the combustor changes significantly. In both cases, two strong shocks originate from the leading edge of the wedge shaped injector. With the non-uniform inflow, two more strong shocks, which are essentially a combination of two weaker shocks originating inside the attached nozzle, enter the combustor. These shocks first reflect off the injector surfaces and then off the upper and lower walls of the combustor. Further downstream, they interact with the two leading edge shocks and the flame. The structure of the flame changed significantly due to its interaction with these two strong shocks. This difference in the flame structures is clearly evident in Figure 5.16.

(a) With a non-uniform inflow

(b) With a uniform inflow

Figure 5.16: DLR combustor: Instantaneous density-gradient contours for the reactive flow
Fluctuations Generated Using SEM

To aid the fuel-air mixing, the SEM (described in §3.5) is used to generate turbulence in the flameholder boundary layers and the hydrogen jets. For the flameholder boundary layers, turbulence generated using the SEM is introduced through an interface between two blocks. Fuel injection ports are treated with a supersonic-inlet boundary condition and turbulence for the hydrogen jets is introduced through these surfaces. Instantaneous density contours highlighting the injector boundary layers, with and without SEM generated fluctuations, are shown in Figure 5.17. The turbulence in the hydrogen jets is visualized in Figure 5.18 using instantaneous hydrogen mass-fraction isosurfaces ($Y_{\text{H}_2}=0.8$) from Cases 1 and 6. Comparing the isosurfaces from both the cases, it is obvious that the hydrogen jets in Case 6, where SEM is used, are more distorted due to higher amounts of turbulence. Also, the hydrogen jets breakup over smaller distances in Case 6, which is evident from the lengths of the isosurfaces from both the cases.

(a) Density-gradient contours with SEM generated fluctuations

(b) Density-gradient contours without SEM generated fluctuations

(c) w-velocity contours with SEM generated fluctuations

(d) w-velocity contours without SEM generated fluctuations

Figure 5.17: DLR combustor: Instantaneous contours highlighting the fluctuations generated in the injector boundary layers using SEM
Figure 5.18: DLR combustor: Instantaneous hydrogen mass-fraction isosurfaces ($Y_{H_2}=0.8$) highlighting the higher turbulence in the hydrogen jets when SEM is used to introduce turbulence into the jets through the injector ports

**Time-Averaged Static Temperature Contours**

Time-averaged static temperature contours for all the cases in Table 5.1 are shown in Figure 5.19. The contours suggest that with each choice, various aspects of the flame (core temperature, flame thickness, and standoff distance) change significantly. These changes in the flame characteristics, due to various choices, are discussed in detail below.

*Case 1, Figure 5.19a:* Grid A, Jachimowski reaction mechanism, and TVD flux reconstruction method are used in this case. The flame observed in this case is lifted, similar to the one observed in §5.1. However, the flame is thicker in this case. The reason for a thicker flame will become more apparent as the subsequent cases are discussed.

*Case 2, Figure 5.19b:* Except for the reaction mechanism, all other methodologies used in this case are same as the ones used in Case 1. Instead of the Jachimowski reaction mechanism, the Ó Connaire reaction mechanism is used to model hydrogen oxidation. There are substantial changes in the flame characteristics. The core of the flame is thicker and hotter for Case 2 compared to Case 1. However, the flame position relative to the injector base is the same as it is in Case 1.

*Case 3, Figure 5.19c:* For this case, the flux reconstruction method is changed from TVD to PPM. All other choices remain the same as in Case 2. Comparing Figures 5.19c, 5.19a, and 5.19b, it is clearly evident that the temperatures in the core of the flame for Case 3 are higher than they are for Case 1 and lower than they are for Case 2. Since PPM is less dissipative compared to TVD, turbulence near the edges of the flame is better
resolved and this improves the fuel-air mixing. This allows for the entrainment of higher amounts of cooler fluid from the freestream into the flame core, which results in lower core temperatures. Once again, the flame position did not change much relative to the injector base.

Case 4, Figure 5.19d: Artificial turbulence is introduced into the injector boundary layers and the hydrogen jets using SEM. This further enhances the fuel-air mixing by increasing the amount of cooler ambient air entrained into the flame. As a result, there is a considerable decrease in the core temperature of the flame compared to Case 3.

Case 5, Figure 5.19e: To resolve the high velocity gradients near the edges of the hydrogen jets better, Grid B is used. Except for the clustering near the edges of the jets, shown in Figure 5.15c, Grid B is essentially the same as Grid A in terms of mesh spacings in the x- and y-directions. To limit the number of cells, the grid is not clustered near the jet boundaries in the spanwise direction. However, within the hole region, the cell size in the spanwise direction is half of what it is for Grid A. The flame position is closest to the base of the wedge for this case, which is evident from the contours. The flame is located 2 mm downstream of the x = 0.120 m location, whereas the flame is 4 mm downstream of the same location for all the previous cases. So enhancing the mixing using SEM has pushed the flame position upstream but it still falls short of the first station.

Case 6, Figure 5.19f: In this case, SEM is used to generate turbulence only for the hydrogen jets (no turbulence generated in the injector boundary layers using SEM). The time-averaged static temperature contours show that the length of the core of the flame is shortened compared to the previous case. However, the region between the shear layers and the hydrogen jets is hottest for this case. This is because flame-propagation toward the base of the injector occurs more frequently in this case, and as a result the time-averaged temperatures in this region are higher by around 150 K. Since fluctuations are not introduced into the injector boundary layers using SEM, the phenomenon of enhanced fuel-air mixing, observed in Case 5, is not observed here. As a result, the core flame temperatures are higher in this case than in Case 5.

Case 7, Figure 5.19g: The non-uniform inflow described in §4.3.1 is used in this case. This allows for the propagation of two strong shocks, originating inside the attached nozzle, into the combustor. These two strong shocks play a crucial role in determining the flame
structure. Compared to all the previous cases, where a uniform inflow was used, the flame thickness in this case is much lower. The overall flame structure is similar to the one observed in §5.1 when the Jachimowski reaction mechanism is used (Figure 5.8b). So it can be said with some confidence that the inflow conditions play a very important role in the prediction of the combustion response in this case.

Figure 5.19: DLR combustor: Time-averaged static temperature contours for all the cases (temperature units in K)
Axial Velocity Line Plots

Figure 5.20 shows axial velocity profiles at six different stations (Stations 1, 2, 3, 4, 6, and 7) downstream of the base of the injector. At Station 1, the station closest to the injector base, none of the cases simulated show good agreement with the experimental results. In the wake of the wedge, axial velocity values are under-predicted in all eight cases. The fact that the predicted flame is thinnest for Case 7 (the case with non-uniform inflow) is clearly evident from the profiles at Stations 1, 2, 3, and 4. At these stations, the width of the region with the velocity deficit is lowest for these two cases. At Station 4, inside the combustion zone, results from Cases 1, 2, and 3 show the closest agreement with experimental data. In the freestream region, except for the cases where the non-uniform inflow is used, all other cases predict nearly the same profiles, which agree well with experiments. At Stations 6 and 7, Case 7 (the cases with non-uniform inflow) shows a velocity deficit inside the flame, which is not observed in any other case. This velocity deficit, which is evident in the experimental profile at Station 7, could be due to the interaction of the strong shocks, which propagate into the combustor from the attached nozzle, with the combustion zone. This interaction decreases the velocity inside the flame, which results in the velocity deficit observed in these two cases.

Static Temperature Line Plots

Static temperature profiles at various stations (Stations 1, 2, 3, 4, 6, and 8) downstream of the injector base are compared with the experimental measurements in Figure 5.21. At Station 1, there is an under-prediction of temperatures in the shear layers compared to experiments. This is because the predicted flame (in all the cases) is detached from the base of the injector. Experimental results show that the temperatures in this region go as high as 1000 K, especially in the shear layers, which could be because of an attached flame. Grids A and B are specifically designed to address this issue. The idea is that, if the turbulence in the shear layers and the hydrogen jets is resolved reasonably well, then this will improve the fuel-air mixing, affect the reaction rates in this region, and change the flame anchoring position. However, this did not change the flame anchoring position significantly. Similarly, none of the other choices (reaction mechanisms, SEM) have the desired effect on the flame position. It is worth mentioning that for Case 6, temperatures in the shear layers are highest. This is because, the localized events where the flame propagates toward the injector backplane are more frequent in Case 6, which
Figure 5.20: DLR combustor: Axial velocity profiles
leads to higher time-averaged static temperature values in this region.

The core flame temperatures increase when the Ó Connaire reaction mechanism is used instead of the Jachimowski reaction mechanism (Cases 1 and 2). This increase from Case 1 to Case 2 is clearly evident in profiles from Stations 2, 3, and 4. When the SEM is used to generate turbulence in the shear layers and the hydrogen jets, higher amounts of cooler air from the freestream are entrained into the combustion zone, which decreases the core flame temperatures. Comparing the line plots for Stations 2, 3, and 4, the peak temperature values for Case 4 are lower compared to all the previous cases where SEM is not used. At Station 4, all the cases over-predict the peak temperature values compared to the experiments. In terms of flame width, the closest match with experiments is shown by the cases where the non-uniform inflow is used. However, even the thinnest flame predicted (Case 7) has a larger width compared to the flame width in the experiments.

**Axial Velocity Fluctuations Line Plots**

The axial-velocity fluctuation profiles are shown in Figure 5.22 at three different axial locations (Stations 1, 4, and 5). At Station 1, the simulations over-predict the fluctuation values in the wake of the wedge and the freestream. In the wake region, the predicted profiles at Station 4 agree well with the experiments, except in Cases 1, 2, and 3, where the peak fluctuation values are over-predicted. At Station 5, predicted profiles from all cases are in good agreement with the experimental values. There is an under-prediction of the turbulence intensity levels in the freestream region due to the absence of freestream turbulence in the simulations.

**Centerline Axial Velocity Line Plots**

Axial velocity profiles along the centerline are compared with the experiment in Figure 5.23. Between x = 0.109 and 0.160 m, all simulations predict a region of recirculation, which was not observed in the experiments. The length of this region is smaller in Case 7 (the case with non-uniform inflow). Further downstream, between x = 0.185 and 0.275 m, Cases 1 through 6 over-predict the axial velocity values compared to experiments. In Case 7, the predicted values are lower compared to Cases 1 through 6 and are closest to the experimental values. This is because of the interaction of the two strong shocks, which are produced inside the attached nozzle, with the flame. This clearly emphasizes the importance of an accurate inflow boundary condition. The fact that the non-uniform
Figure 5.21: DLR combustor: Static temperature profiles
inflow changed the flame structure substantially further asserts the need for an accurate inflow boundary.

**Lower-Wall Pressure Line Plots**

The predicted pressure profiles along the lower wall of the combustor are compared with experimental measurements in Figure 5.24. Profiles from Cases 1 through 6 (the cases with uniform inflow) follow a particular pattern, which is visually different from the pattern followed by the profile from Case 7 (the case with non-uniform inflow). This reiterates the fact that the shock structures produced when uniform and non-uniform inflows are used are different.

*Cases 1 through 6:* At $x \approx 0.109$ m, shock produced from the leading edge of the injector reflects off the lower wall. The profiles show a steep increase in the pressure, which is due to this reflection of the leading edge shock. At $x \approx 0.127$ m, the shock produced off the lower wall at the inflow of the combustor reflects off the injector surface and then impinges on the lower wall. The little spike in pressure observed at this location is because of this shock. The interaction of the supersonic freestream with the flame surface produces an
expansion fan, which interacts with the boundary layer on the lower wall at $x \approx 0.155$ m. This interaction results in a steep decrease in pressure, which is evident in the profiles.

**Case 7**: Profiles in both cases follow each other very closely. Downstream of the injector base, since the shape of the flame is different from the one observed in Cases 1 through 6, the locations where the shocks and expansion waves impinge on the lower wall are different. Also, the shape of the flame has an effect on the strength of the expansion fan. As a result of the difference in the shock strengths and reflection locations, the magnitudes and locations of pressure rises are also different.

However, none of the predicted profiles are in good agreement with the experiments. This could be due to the same two reasons mentioned before. Though the non-uniform inflow is a more accurate representation of the experimental inflow conditions, it can be said that the inflow boundaries (uniform and non-uniform) probably do not accurately represent the experimental inflow conditions. As a result, the shock structure propagating into the combustor from the nozzle, the boundary layer thicknesses at the entrance of the combustor, and the overall shock structure inside the combustor could be markedly different from the experiments. All these factors could bring about a significant change in the overall flame shape and shock reflection locations, which could be the reasons why the peaks in the predicted profiles shifted downstream compared to the measured profiles.
Figure 5.23: DLR combustor: Centerline axial velocity
Figure 5.24: DLR combustor: Static pressure along the lower wall
Chapter 6

Subgrid Closures for Filtered Species Production Rates

In the present chapter, several SGS combustion models that do not assume a flame structure are used to calculate the filtered species source terms: laminar chemistry (turbulence-chemistry interactions ignored) model, three different Partially Stirred Reactor (PaSR) type SGS models, and one Scale-Similarity (SS) type SGS model. Reactive flows through: the DLR combustor and the UVa-A combustor are simulated as test cases.

6.1 Grid, Initial and Boundary Conditions

6.1.1 DLR Combustor

For the DLR combustor, Grid B (§5.2.1) is used, and all simulations are initialized using the statistically steady state of Case 7 from §5.2.4. Boundary conditions imposed are also the same as in Case 7, where the non-uniform inflow is used for the combustor inflow and the SEM is used to force unsteadiness in the hydrogen jets.

6.1.2 UVa-A Combustor

The meshes used to represent the Mach 2 nozzle and the combustor contain around 16 million and 33 million cells, respectively. The average cell size in the isotropic regions is 0.00035 m, and the normal spacing at the walls is $5 \times 10^{-6}$ m. The multi-block
decomposition of the combustor mesh and topology around the ramp injector are shown in Figure 6.1.

![Multi-block decomposition](image1.png)

(a) Multi-block decomposition

![Mesh topology around the ramp injector](image2.png)

(b) Mesh topology around the ramp injector

Figure 6.1: UVa-A combustor: Mesh

The flow through the Mach 2 nozzle is simulated separately using RANS techniques, and the steady state outflow profile is then used as the mean inflow condition for the LES/RANS calculations involving the UVa-A combustor. The procedure described in §4.3.2 is used to account for an observed degree of flow asymmetry in the facility nozzle (reported by planar CARS temperature diagnostics). The wall temperature is set at 600 K except for a narrow region just downstream of the injector, where it is set to 1000 K. In this region, a zirconia coating is used to aid in flameholding, and the value of 1000 K is arrived at using experimental thermocouple data. Flow through the injector channel is
simulated as part of the overall mesh used in the RANS calculations. Since the flow at the exit of the injector port is supersonic, the flow inside the injector channel is decoupled from the core flow in the LES/RANS simulations. The exit profiles from the injector channel are then extracted from the RANS results and interpolated to the finer mesh used in the LES/RANS calculations. At the outflow, pressure in the ghost cells is set to ambient pressure where the flow is subsonic, and is extrapolated from the interior when the flow is supersonic.

6.2 Reaction Mechanisms

To model hydrogen oxidation, the reaction mechanism of Ó Connaire et al. [5] is used for the DLR combustor, while the Jachimowski [2] and Burke et al. [6] reaction mechanisms are used for the UVa-A combustor. Details of these reaction mechanisms are presented in Appendix A.

6.3 Time Advancement

6.3.1 DLR Combustor

As in §5.2.3, all LES/RANS calculations performed in the current chapter are evolved at a constant time step of $1 \times 10^{-7}$ seconds, and to reach a statistically steady state, the flow is first allowed to evolve for two flow-through-times. Time averages are then collected for four flow-through-times. Results presented in the form of line-plots are span-averaged over the entire spanwise length of grid, which spans across five fuel injector holes.

6.3.2 UVa-A Combustor

For the UVa-A combustor, the flow is allowed to evolve at a constant time step of $1.5 \times 10^{-7}$ seconds for two combustor-transit-times and then statistics are collected for five combustor-transit-times. A combustor-transit-time is defined as the time required for the flow to traverse through the combustor section. The combustor length is 0.375 m and the free-stream velocity is approximately 1035 m/s, which means the combustor-transit-time is approximately 0.0003623 seconds.
6.4 *A Priori* Analyses

6.4.1 Model Constant Estimation

To investigate the relative merits of the models described in §2.2.6 in accounting for the effects of subgrid fluctuations on chemical production rates, several *a priori* analyses were conducted based on data extracted from a fine-mesh LES/RANS simulation of the reactive flow in the UVa-A combustor. Specifically, species density, temperature, velocity, viscosity, and cell volume values were extracted from 23 discrete locations distributed within the flame at four y-z planes (x/H = 3, 6, 12, and 18) over a period of 2200 time steps (approximately one combustor-transit-time). The total number of data sets is thus 202400 (23 x 4 x 2200). Each data set consists of information from all the cells within a 4 cell x 4 cell x 4 cell volume surrounding each discrete location. It is possible to filter the data at a coarser mesh level to obtain enough information to evaluate the PaSR(0), PaSR(SS), and SS models, with the exact filtered data at the coarser mesh level being the ‘truth model’ to which the others are compared with. The PaSR(1) model involves the solution of transport equations and is not amenable to this type of analysis.

A volume-weighted filtering operator is defined as

\[
\bar{Q} = \frac{\sum_{k=1}^{N} \Omega_k Q_k}{\sum_{k=1}^{N} \Omega_k}
\]  

(6.1)

where \( \Omega_k \) is the volume of cell \( k \) and \( Q_k \) is the fine-mesh property at cell \( k \). Two merit functions are used to establish model performance. One is an \( L^2 \) norm of the species production rates, defined as

\[
||\vec{\omega}|| = \left( \sum_s (\dot{\omega}_s(\rho_s,T))^2 \right)^{1/2}
\]  

(6.2)

and the other is a measure of the temperature change per unit time resulting from constant-volume heat release, defined as

\[
\Delta T = - \frac{\sum_s (h_s(T) - R_sT)\dot{\omega}_s(\rho_s,T)}{\sum_s \rho_s(C_{p,s}(T) - R_s)}
\]  

(6.3)
A comparison would involve equating the filtered merit function with the one defined using a specific model (subscript ‘mod’). For example, one compares
\[ \| \vec{\omega} \| = \left( \sum_s (\dot{\omega}_s(\rho_s, T))^2 \right)^{1/2} \] with \[ \| \vec{\omega} \| \text{mod} = \left( \sum_s (\dot{\omega}_s(\rho_s, T) \text{mod})^2 \right)^{1/2}. \] To compare filtered and modeled merit functions, we calculate correlation coefficients and slopes according to the following:
\[ \text{corr}(a, b) = \frac{\text{cov}(a, b)}{\left( \text{cov}(a, a) \text{cov}(b, b) \right)^{1/2}}, \quad \text{slope}(a, b) = \frac{\text{cov}(a, b)}{\text{cov}(a, a)} \] (6.4)
with the covariances defined by
\[ \text{cov}(a, b) = \sum_k f \left( \frac{a_k}{b_{k,LC}} \right) a_k b_k - \left( \sum_k f \left( \frac{a_k}{b_{k,LC}} \right) a_k \right) \left( \sum_k f \left( \frac{a_k}{b_{k,LC}} \right) b_k \right) \] (6.5)
Here, \( f \left( \frac{a_k}{b_{k,LC}} \right) \) is a normalized probability density function for the ratio of the filtered merit function \( (a) \) to the modeled value computed using the ‘laminar chemistry’ assumption \( (b_{LC}) \).

Representative (non-normalized) probability density functions for the production-rate \( L^2 \) norm and temperature change metrics are shown in Figure 6.2. The distribution functions are largest in the interval from zero to one, peaking near one, before decaying to zero as the ratio of filtered to laminar-chemistry values increases. This implies that subgrid fluctuations are more likely to reduce species production rates and heat release but that there are a number of regions within the flame where the fluctuations either have no effect or that they enhance species production rates. The fact that the \( L^2 \) norm of the production rates is non-negative disallows the probability of fluctuations forcing a sign change in this metric, but an examination of the probability density functions for individual source terms (Figure 6.3) indicates that fluctuations may also induce sign-reversal for some source terms. The PaSR(0) model cannot account for enhancement or sign-reversal, whereas the PaSR(SS) model can account for enhancement, but not sign-reversal. Only the SS model could potentially capture both effects.

Figures 6.4 and 6.5 show the results of the model correlation analysis. The correlation coefficient and slope for each of the models (relative to the filtered data) is plotted versus the model constant for the production-rate \( L^2 \) norm and temperature change metrics. Optimal model performance is a value of unity for both the correlation coefficient and the slope. The results were obtained by computing the correlation coefficients and slopes for
Figure 6.2: UVa-A combustor: Probability distribution function: production-rate $L^2$ norm and temperature change metrics
Figure 6.3: UVa-A combustor: Probability distribution functions: species production rates
Figure 6.4: UVa-A combustor: Correlation coefficient and slope versus model constant: temperature change metric
Figure 6.5: UVa-A combustor: Correlation coefficient and slope versus model constant: production-rate $L^2$ norm metric
each data plane, then averaging the values. Figure 6.4, corresponding to the temperature change metric, shows that the correlation coefficient is invariant (as expected) with respect to model constant for the PaSR(SS) model and is weakly dependent on the model constant for the SS model. The correlation coefficient increases as the model constant decreases for the PaSR(0) model, implying that the limiting case of the model constant being zero (equating the model to ‘laminar chemistry’) is optimal for this model. Only the SS model yields a correlation coefficient better than ‘laminar chemistry’. This occurs for model constants up to 1.3, with the peak value of 0.983 occurring at a model constant of 0.68. The correlation coefficient for the PaSR(SS) model is slightly less than that of ‘laminar chemistry’ (0.969 versus 0.971). Optimal values for the slope occur at \( c_1 = 1.19 \) for the SS and at \( c_1 = 1.10 \) for the PaSR(SS) model. For the range of model constants considered (0.25 to 1.5), the slope values are consistently below unity for the PaSR(0) model, implying that the effect of the PaSR(0) model will be to reduce heat release consistently, relative to the filtered data and to the other optimized models. In contrast, the slope value for ‘laminar chemistry’ is larger than unity (1.1), implying that this model will increase heat release, relative to the filtered data.

Figure 6.5 presents similar results for the production-rate \( L^2 \) norm metric. Here, the best correlation coefficient is provided by the PaSR(SS) model (0.965), followed by the SS model for model constants between 0.25 and 0.65. The ‘laminar chemistry’ model also provides an acceptable correlation (0.958), and the PaSR(0) model generally correlates worse than the others. An optimal slope value is realized by the PaSR(0), SS, and PaSR(SS) models at model constants of \( c_1 = 0.76 \), \( c_1 = 0.874 \), and \( c_1 = 1.20 \), respectively. Again, the ‘laminar chemistry’ slope value (1.55) exceeds unity, implying that this model will over-estimate the production rates of major species.

The general conclusion of the \textit{a priori} analysis is that the SS and PaSR(SS) models have the potential to out-perform the ‘laminar chemistry’ model but that the PaSR(0) model, as currently formulated, will likely lead to lower levels of heat release. Considering only the slope data and averaging among all values, an ‘optimal’ model constant is 0.99 for the PaSR(SS) model, 1.2 for the SS model, and 0.73 for the PaSR(0) model. For all cases shown later, however, the model constant \( c_1 \) is assigned a value of unity.
6.4.2 Time- and Length-Scale Comparisons for PaSR(1)

Various models exist in literature which define the volume fraction $\gamma^*$ and the diffusion time-scale $t_m$, three of which are defined in §2.2.6: Giacomazzi et al. [13], Fureby et al. [73, 12], and EDC [74]. Figure 6.6 plots the three proposals for $\gamma^*$ versus $Re_\Delta$. To obtain this plot, $u_{sgs}$ is varied from 1 m/s to 100 m/s and the kinematic viscosity and filter width are set to $10^{-5} \text{ m}^2/\text{s}$ and 0.5 mm, respectively. These values are representative of those obtained in the UVa-A combustor. It is obvious that each proposal interprets the fine-scale volume fraction in a different manner. In Fureby’s proposal, the volume fraction of fine-scale structures approaches one as $Re_\Delta$ increases. This implies a dramatic increase in the number density of Kolmogorov eddies, as their sizes diminish as the Reynolds number increases. In the EDC model, the volume fraction decreases as the Reynolds number increases so that the volume of fine-scale structures scales as $\Omega^* \sim (\Delta l_k)^{3/2}$ - the cube of the geometric average of the filter width and the Kolmogorov scale.

![Figure 6.6: PaSR(1): Fine-scale volume fraction for different models](image)

The time-scale values are plotted versus $Re_\Delta$ in Figure 6.7 as is the product $(1 - \gamma^*)t_m$.
Figure 6.7: PaSR(1): Mixing time-scales for different models

Figure 6.8: PaSR(1): Product of mixing time-scale and coarse-scale volume fraction for different models
in Figure 6.8. The Schmidt number is assumed to be 0.5, which is a common practice for hydrogen-air combustion. Overall, the results for the key parameter $(1 - \gamma^*)t_m$ are relatively close, with Fureby’s PaSR and the EDC model being nearly equivalent. The value of $(1 - \gamma^*)t_m$ is consistently higher for the PaSR(1) model, implying that reactions and time-dependence will play a more dominant role, relative to diffusion, in the solution of the fine-scale sub-system.

6.5 Results

Reactive flows through the DLR and UVa-A combustors are simulated using the five different subgrid closures for calculating the filtered species source terms, namely: laminar chemistry, PaSR(0), PaSR(1), PaSR(SS), and SS, which are described in §2.2.6. The baseline simulations use the ‘laminar chemistry’ subgrid closure; in all subsequent simulations only the subgrid closure for calculating the filtered species production rates is changed. This means that any changes in the predictions are due to the choice of this subgrid closure. Results from all these simulations are compared with the data available from both the experiments, and are presented below.

6.5.1 DLR Combustor

Though static temperature measurements from experiments are available only at Stations 1, 4, and 8; profiles from simulations are presented at six different stations (1,2,3,4,6, and 8), for the purpose of qualitatively comparing the predictions from different models at each of these stations. At Station 1, all models predict nearly the same values, which are considerably lower than the values measured in the experiments. The higher temperatures observed in the experiments at this station suggest that the flow is reactive here, especially in the shear layers where the measured temperatures are as high as 1000 K. Since the flow predicted by all the models is non-reactive at this station, it is not surprising that the predicted profiles from all simulations are nearly the same. At Station 2, PaSR(0) predicts the highest peak value for temperature, which is not obvious since ‘laminar chemistry’ is expected to predict highest reactivity at any given point. At Stations 3, 4, and 6; static temperature predictions from all models are nearly the same. At Station 6, all models overpredict the static temperature values; the experimental profile at this station suggests that the flame is thinner and cooler. In the last station (Station 8), profiles predicted
by all closures closely follow each other except PaSR(0), which predicts the lowest peak value of temperature. The experimental profile at this station shows that the peak value measured ($\approx 1500$ K) is much lower than the predicted peak values, ($\approx 2000$ K for all models except PaSR(0), which predicts a peak value of $\approx 1800$ K).

Figure 6.9: DLR combustor: Static temperature profiles from simulations and experiments at various x-locations.

Axial velocity profiles at Station 1,2,3,4,6, and 7 predicted by all models are shown.
Figure 6.10: DLR combustor: Axial velocity profiles from simulations and experiments at various x-locations downstream of the base of the flameholder
in Figure 6.10, and are compared with experimental profiles where available. Profiles predicted by PaSR(0) at Station 4 and 6 clearly stand out, which show that the axial velocity values inside the flame are under-predicted by PaSR(0). At all other stations the values predicted by all models are very much the same.

Centerplane static temperature contours from all five simulations are shown in Figure 6.12. The differences in the flame structure and temperature are very subtle and not significant. Between x=0.125 m and x=0.14 m, PaSR(SS) and SS predict the lowest flame temperatures. Compared to the flame core position predicted by ‘laminar chemistry’, the position predicted by PaSR(0) is closer to the base of the flameholder. This explains why at Station 2, the peak temperature predicted by PaSR(0) is the highest. Downstream of x=0.25 m, the flame temperatures are lowest when PaSR(0) is used, which is also reflected in the static temperature line plots. Except for these minor differences, the flames predicted by all models are very similar to each other. The trend of decrease in flame temperatures downstream of x=0.25 m, when PaSR(0) is used, is expected to be seen through out the flame. However, a decrease in the species production rates due to the subgrid closures never materialized into lower flame temperatures. Overall, the influence of various closures on the flow through the DLR combustor is not as pronounced as expected. It can be said that, except at a couple of stations, all models yield nearly identical results.
Figure 6.11: DLR combustor: Axial velocity profiles along the geometric centerline (top) and static pressure distributions along the lower wall (bottom)
Figure 6.12: DLR combustor: Centerplane temperature contours
6.5.2 UVa-A Combustor

Figure 6.13 shows a snapshot of temperature along the combustor centerplane and at various cross-planes downstream of the ramp base ($x/H = 6$, $12$, and $18$). The flame is anchored in the low-momentum region just downstream of the fuel injector and propagates downstream along the outer edges of the counter-rotating vortex pairs emanating from the ramp injector. As these vortices break down, the reaction zone becomes more entangled but still remains nominally in the thin reaction zone (or flamelet) regime.

The performance of each of the subgrid-scale closure models is assessed for the UVa-A combustor in this subsection. A solution is first obtained for the Jachimowski reaction model. This solution is then used as the starting point for additional simulations that employ the Burke et al. hydrogen oxidation model with several subgrid-scale closures.

Wall pressure distributions in Figure 6.14 indicate that all models generally capture the experimental trends but under-predict pressure levels near the injector. This is a consequence of an under-prediction of the degree of volumetric expansion of the plume.
near the injector. The Jachimowski and PaSR(0) predictions are the worst in this regard, indicating that these models produce less heat release near the injector.

Figure 6.14: UVa-A combustor: Wall pressure distributions

Figures 6.15 and 6.16 compare mean and \textit{rms} temperature distributions with CARS data. To arrive at these distributions, the computational data values are interpolated to the CARS data points. A triangulation of the data points is then performed using Tecplot to yield the planar images shown. The scales for each plane are different to highlight subtle variations in the solutions provided by each of the subgrid-scale models.
Figure 6.15: UVa-A combustor: Temperature contours at different axial stations compared with CARS data (Contour ranges different for different axial locations); top row: x/H = 6, middle row: x/H = 12, and bottom row: x/H = 18
Figure 6.16: UVa-A combustor: \textit{rms} temperature contours at different axial stations compared with CARS data (Contour ranges different for different axial locations); top row: x/H = 6, middle row: x/H = 12, and bottom row: x/H = 18
Comparing the baseline ‘laminar chemistry’ Jachimowski and Burke et al. solutions, the temperature pattern is better predicted by the Jachimowski model, particularly at x/H = 6 and 12. All models under-predict the degree of plume expansion at x/H=12 though agreement with CARS data improves at x/H = 18. The PaSR(0) model under-predicts the temperature at x/H = 12 and x/H = 18. The PaSR(1) and SS models yield mean temperature predictions that are similar to the Burke et al. ‘laminar chemistry’ model. The PaSR(SS) mean temperature prediction is similar to PaSR(0) at x/H = 6 and x/H = 12 but is closer to the Burke et al. ‘laminar chemistry’ prediction at x/H = 18. Temperature $rms$ distributions generally mirror the mean trends in that models that yield higher temperature levels also yield higher $rms$ temperature values. Among the models, the PaSR(SS) and Jachimowski provide the best visual comparison with the CARS distributions.

Figures 6.17 and 6.18 compare mean and $rms$ oxygen mole-fraction distributions with CARS data. Figure 6.17 shows that all models under-predict the vertical extent of the reaction plume at x/H = 12 but agree well with the data at x/H = 6 and x/H = 12. Differences among the models are most pronounced at x/H = 18. Oxygen mole fraction levels are higher in the core of the plume for PaSR(0), echoing the diminished reactivity for this model indicated in the temperature distributions. The PaSR(1), SS, and Burke et al. ‘laminar chemistry’ models again give similar predictions. The PaSR(SS) and Jachimowski models predict similar levels of reactivity at all stations, though the PaSR(SS) plume at x/H = 18 is not as symmetric as the others. The $rms$ mole fraction distributions (Figure 6.18) show that all models appear to be in good quantitative agreement with CARS measurements, with the Jachimowski and PaSR(SS) models again providing the best visual comparisons.
Figure 6.17: UVa-A combustor: Mean oxygen mole-fraction contours at different axial stations compared with CARS data (Contour ranges different for different axial locations); top row: x/H = 6, middle row: x/H = 12, and bottom row: x/H = 18
Figure 6.18: UVa-A combustor: $rms$ oxygen mole-fraction contours at different axial stations compared with CARS data (Contour ranges different for different axial locations); top row: $x/H = 6$, middle row: $x/H = 12$, and bottom row: $x/H = 18$
Model Error Analysis

The performance of each model is assessed by quantifying the errors from simulation using the experimental CARS or SPIV data. The formula used to estimate the overall error at each axial plane is shown below:

$$\varepsilon_k = \frac{\sum_{k=1}^{N} |Q_{k, \text{LES}} - Q_{k, \text{CARS, SPIV}}|}{\sum_{k=1}^{N} Q_{k, \text{CARS, SPIV}}} \times 100$$  \hspace{1cm} (6.6)

where $N$ is number of CARS or SPIV data points. Figures 6.19a-6.19c show this error metric for each of the variables and each of the models for $x/H = 6, 12,$ and $18$. With the exception of hydrogen mole fraction (which shows some inconsistent trends in the experimental data), mean errors are less than 20% and errors in the $\text{rms}$ quantities are between 20% and 50%. Errors in the velocity magnitude (only measured at $x/H = 12$) are around 19% for all models. The overall error levels diminish for the downstream stations. The degree of error variation with respect to the subgrid-scale model is not large for any variable.

To attempt to quantify model performance more precisely, we consider a metric that compares a model’s accuracy (relative to measured data) with respect to a baseline model. The Burke et al. ‘laminar chemistry’ solution is considered as the baseline, and the metric is defined as

$$P_{\text{model}} = \sum_{k=1}^{Nv,Np} m(\varepsilon_{k, \text{baseline}} - \varepsilon_{k, \text{model}}) \quad \text{and} \quad m(\alpha) = \begin{cases} 1, & \alpha > 0.25 \\ -1, & \alpha < -0.25 \\ 0, & -0.25 < \alpha < 0.25 \end{cases}$$  \hspace{1cm} (6.7)

Here, $Nv$ is the number of variables and $Np$ is the number of data planes. The maximum possible score for a model is 25, meaning that for all variables and all planes, the errors are less than the baseline. The minimum possible score is -25. Model ‘neutrality’ is accounted for by adopting a zero score for absolute error percentage differences of less than 0.25.

Scores for each of the models are shown in Table 6.1. It is clear from this analysis that there is no truly superior subgrid-scale model among the ones tested. The ‘laminar
chemistry' Jachimowski model and the scale similarity subgrid-scale model provide the most improvement, relative to the baseline, but the degree of improvement is quite modest.

Table 6.1: Subgrid closures for filtered species production rates: Scores indicating the performance of each model

<table>
<thead>
<tr>
<th>Model</th>
<th>Score (Maximum of 25)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jachimowski 'laminar chemistry'</td>
<td>5</td>
</tr>
<tr>
<td>Burke et al. 'laminar chemistry'</td>
<td>0 (baseline)</td>
</tr>
<tr>
<td>Burke et al. PaSR(0)</td>
<td>-5</td>
</tr>
<tr>
<td>Burke et al. PaSR(1)</td>
<td>2</td>
</tr>
<tr>
<td>Burke et al. PaSR(SS)</td>
<td>2</td>
</tr>
<tr>
<td>Burke et al. SS</td>
<td>5</td>
</tr>
</tbody>
</table>

**Computational Cost**

Table 6.2 shows the CPU time required for each time iteration (6 sub-iterations) and the expense relative to the 'laminar chemistry' subgrid closure for all of the subgrid closures used in the present study. Relative to 'laminar chemistry', PaSR(0) is the least expensive. This is obvious since the formulation requires the same number of computations as 'laminar chemistry'. PaSR(SS) and SS cost nearly the same, as both involve calculation of the species production rates three times ('laminar chemistry' and PaSR(0) require one time calculation of species production rates). PaSR(1) is the costliest, nearly 30 % costlier than 'laminar chemistry'. The model requires solving an additional system of equations (nine transport and one energy equation for the Ó Connaire et al. and Burke et al. reaction mechanisms), which means one additional calculation of Jacobian, one additional calculation of species production rates, and solving the resulting system of equations; all this adds up to the nearly 30 % additional CPU time. From a cost-benefit perspective, none of the models tested are a significant improvement over 'laminar chemistry' for the cases tested and the mesh resolutions employed.
Table 6.2: CPU time required for each iteration of time for various subgrid closures

<table>
<thead>
<tr>
<th>Subgrid closure</th>
<th>CPU time</th>
<th>Relative expense</th>
</tr>
</thead>
<tbody>
<tr>
<td>‘Laminar chemistry’</td>
<td>≈ 16.50 s</td>
<td>-</td>
</tr>
<tr>
<td>PaSR(0)</td>
<td>≈ 16.50 s</td>
<td>0 %</td>
</tr>
<tr>
<td>PaSR(1)</td>
<td>≈ 21.64 s</td>
<td>+31.15 %</td>
</tr>
<tr>
<td>PaSR(SS)</td>
<td>≈ 19.77 s</td>
<td>+19.81 %</td>
</tr>
<tr>
<td>SS</td>
<td>≈ 19.50 s</td>
<td>+18.18 %</td>
</tr>
</tbody>
</table>

Inferences

The subgrid closure models tested in the present chapter generally decrease the magnitude of the species production rates, relative to the ‘laminar chemistry’ closure. In this regard, PaSR(0) is the most aggressive, as it directly incorporates a time-scale characteristic of subgrid mixing as a rate-limiting factor. A similar time-scale is utilized in PaSR(1) to govern diffusion-induced transport between fine and coarse-scale structures. The effects of this time-scale in limiting chemical production are more indirect in PaSR(1), as advection and temporal changes also impact the balance. PaSR(SS) and the scale-similarity model do not incorporate a mixing time-scale. Here, the degree of ‘unmixedness’ found within the SGS scales is estimated by grid-filtering resolved-scale data. These models depend directly on reactive-scalar behavior and are indirectly impacted by modeled turbulent mixing near the grid scale. Though all models decrease species production-rates on the average, they do not have a proportional impact on heat release or flame temperatures. One reason may be that compensating effects (enhanced turbulent diffusion toward the flame front) may counteract the effect of the closure. Another reason, motivated by the results of the *a priori* analysis, is that overall heat release is less sensitive to the neglect of SGS effects than, for example, production rates of the major species. One more reason may be the mesh resolution, which is fine enough in the isotropic regions of the combustor to capture a laminar flame in two or three mesh cells. Though this level of resolution is insufficient to resolve the internal flame structure, the response of the ‘flamelets’ to turbulence near the grid scale may be captured accurately enough to render mean-flow predictions relatively insensitive to modeled SGS effects.

It is important to point out that the reactive flows in the DLR and UVa-A combustors
are characterized by two different type of flow-fields. In the DLR combustor, the mixing process is dominated by large, Kelvin-Helmholtz - type roller structures that originate at the trailing edges of the flameholder. In the UVa-A combustor, mixing is dominated initially by axial vortex pairs generated as the flow spills around the edges of the ramp injector. These structures rapidly break down into small eddies, leading to a higher degree of micromixing and lower turbulence intensities than in the DLR case. This fundamental difference in the flow fields could be a reason why the PaSR(0) closure impacts the UVa-A combustor more than the DLR combustor. The turbulence intensity remains high for the DLR combustor, as the large structures do not break down quickly. Chemical time-scales are rate-limiting for the majority of the DLR combustor, whereas mixing time-scales are rate-limiting for the more downstream stations in the UVa-A combustor.
Figure 6.19: UVa-A combustor: Percentage of errors compared to CARS or SPIV data
Chapter 7

Ethylene Fueled Cavity Flameholder

The Hypersonic Technology (HyTech) program [93], initiated in 1995, was intended to develop a hydrocarbon-fueled scramjet engine for military, transport, and space flight (air-breathing stage) purposes. The X-51A Scramjet Engine Demonstrator (SED), which was developed as part of the HyTech program, uses ethylene for initial ignition and later makes a transition to the hydrocarbon based JP-7 fuel. The X-51A SED performed its first fully successful 240 second flight test on 14 August 2012, increasing the interest in developing hydrocarbon-fueled scramjet engines. Hydrocarbon fuels are preferred over hydrogen due to their high density (which means lower fuel tank volume), ease of handling, and increased safety [94, 93]. However, the ignition delay times for long chain hydrocarbons are large; meaning, they pose significant challenges when used as fuel in scramjets, where the fuel-residence times are often less than a millisecond. These challenges include, but are not limited to, ignition of the fuel (which means formation of sufficient number of free radicals to initiate the chain reactions) and flameholding.

Use of cavity flameholders as a way to increase the fuel-residence times and fuel-air mixing was first proposed by [95]. They were first used in a joint French/Russian venture, where a hydrogen fueled, dual-mode scramjet was tested [96]. Later experiments [97, 98, 99] showed that use of a cavity after the ramp injector significantly improves the combustion efficiency of hydrocarbon fuels in scramjets. A detailed description of various cavity flameholder designs and their performances is given in [100]. In the current chapter, reactive flow through an ethylene-fueled cavity flameholder is simulated using a hybrid LES/RANS method. The cavity flameholder considered is the UVa-E combustor (described in §4.2.2).
7.1 Grid

The grid representing the isolator, combustor, and extender sections, shown in Figure 7.1, is comprised of 11,307 blocks and 59,825,632 cells. The average mesh spacing in the mixing region is 0.0003 m, and the minimum mesh spacing at all solid walls is $5 \times 10^{-6}$ m. The grid has circular topologies rendered for all rows of injection ports available in the actual configuration; however, for the case considered in the present study, ethylene is injected only through the most upstream row. So, except for the most upstream row of injector ports, all others are treated as walls.

Figure 7.1: UVa-E combustor: Grid topology
7.2 Reaction Mechanisms

To model ethylene-air chemical kinetics, initial simulations used a modified version of the 14-species reaction mechanism of Gokulakrishnan et al. [7] (details listed in Appendix A), which resulted in a flame blowout. The later simulations use the Taitech/Princeton reduced ethylene kinetics model, TP-2 [64, 63], which consists of 22-species. The TP-2 mechanism is available in the form of a Fortran subroutine, which takes pressure, temperature, and species mass-fractions as input and returns the species production rates as output. In its current implementation as part of NCSU’s REACTMB, species production rates and their Jacobians are calculated using this subroutine. The Jacobians are calculated by repeatedly calling the subroutine with small perturbations in the input quantity with respect to which the derivative is to be calculated. These repeated calls to the subroutine increase the overall computational cost associated with using the TP-2 reaction mechanism. Also, the sum of the production rates of all species, as calculated by the subroutine, is not identically zero. It was observed that this imposed limitations on the global time-step that can be used in the LES/RANS simulations. Enforcing the condition that the sum of species production rates (for non-inert species) is zero (enforced as shown in Equation 7.1) relaxed the limitation on the time-step, but not significantly.

\[ \dot{\omega}_{s,\text{adjusted}} = \dot{\omega}_{s,\text{TP-2}} - Y_i \sum_i \dot{\omega}_{i,\text{TP-2}} \]  

(7.1)

where \( s \) is one of the non-inert species and the summation in the second term is over the number of non-inert species. In the LES/RANS simulations described in the current chapter, the ‘laminar-chemistry’ subgrid closure is used to calculate the filtered species production rates.

7.3 Initial and Boundary Conditions

Converged RANS solutions are used to initialize the LES/RANS simulations. Non-reactive flow through the UVa-E combustor is first simulated using RANS techniques. The steady state non-reactive RANS solution is used to initialize the reactive RANS simulation (with the 14-species reaction mechanism), where reactions are initialized using a spatial ignition source placed in the low momentum region behind the cavity leading edge. The reactive RANS solution (with the ignition source in place) is allowed to reach steady state, which
is then used to initialize the reactive LES/RANS simulations, where the ignition source is no longer in place.

As in §6.1.2, the flow through the Mach 2 nozzle is simulated separately using RANS techniques, and the steady state outflow profile from the nozzle simulation is used as the mean inflow condition for the UVa-E combustor in the LES/RANS simulations performed in the present chapter. Once again, the procedure described in §4.3.2 is used to account for the flow asymmetry observed in the Mach 2 nozzle. The wall temperatures are set at 600 K everywhere. To simplify imposing a fixed back pressure boundary condition at the exit plane of the extender, a dump region is attached to the exit plane. The boundary conditions imposed on various planes of this dump region are shown in Figure 7.2. Ethylene is injected through the most upstream row of injector tubes; a separate multi-block mesh is generated for one of these tubes, and conditions at the exit plane of the injector tube are calculated using RANS techniques. These exit conditions are then imposed as inlet conditions on the injector ports of the combustor. Also, SEM (described in §3.5) is used to generate turbulence at the inflow plane of the UVa-E combustor.

### 7.4 Inflow Forcing

The influence of turbulence in the boundary layers can be significant for internal flows with shocks [101]. The presence of a turbulent boundary layer in the isolator section will help in predicting accurate shock-wave-boundary layer interactions. To this end, the SEM (described in §3.5) is used for introducing turbulence in the boundary layers at the inflow plane of the UVa-E combustor. In Figure 7.3, the development of this turbulence is visualized using centerplane w-velocity and density gradient contours of the flow in the isolator section of the UVa-E combustor.

### 7.5 Time Advancement

The LES/RANS simulations performed using the 14-species reaction mechanism are evolved at a constant time step of $1.0 \times 10^{-7}$ seconds. The flow is allowed to evolve for two combustor-transit-times ($2 \times 0.0003623$ seconds) to wash-out the transience associated with the steady state RANS solution, which is used as the initial condition for the LES/RANS simulations. Statistics are then collected for nearly six combustor-transit-times. With
the TP-2 mechanism, due to the stability issues described in §7.2, a smaller time-step of $0.5 \times 10^{-7}$ seconds is needed to keep the solution stable. Once the solution reached a statistically steady state, statistics are collected for nearly four and half combustor-transit-times.

### 7.6 Results

Statistics, at Stations 1, 2, and 3, are collected every 100 iterations. One set of statistics is referred to as a frame, and the instantaneous contours shown in the current section correspond to a particular frame. The time-averaged data is calculated by averaging the data from all the frames.
When the 14-species reaction mechanism is used to model ethylene-air kinetics, the flame is statistically stable for nearly four combustor-transit-times, after which there is a steady decrease in the heat release ultimately resulting in a flame blowout. In Figures 7.4, 7.5, and 7.6, this process of flame blowout is visualized using instantaneous cross-plane contours of various quantities at Stations 1, 2, and 3 (see Figure 4.5). At all three stations, the steady decrease in the flame temperatures with time is clearly visible in Figures 7.4a, 7.5a, and 7.6a. As the flame temperatures decrease, there is a decrease in the consumption of ethylene, which is evident in Figures 7.4b, 7.5b, and 7.6b. Also, mass-fractions of CO$_2$, CO, and H$_2$O follow the same trend as the flame temperatures. At Stations 2 and 3, at t=0 seconds, the flame propagates along one of the side walls (first rows of Figures 7.5a and 7.6a). As will be shown in §7.6.2, this straining in the flame along the side wall is not observed when the TP-2 reaction mechanism is used.

In Figure 7.7, time-variations in the predicted profiles (each profile corresponds to
data time-averaged over 20 frames) of H$_2$O temperature, H$_2$O column-density, and CO$_2$ column-density are compared with experimental measurements. There is a steady decrease in the magnitudes of all the three quantities, indicating that the heat release at each of the stations is steadily decreasing with time.

Figure 7.4: UVa-E combustor: Time-evolution of the instantaneous solution at Station 1 when the 14-species reaction mechanism is used (cross-plane contours; first row: t=0 seconds, second row: t=0.00075 seconds, third row: t=0.0015 seconds, fourth row: t=0.00224 seconds; each column corresponds to contours of a particular variable)
Figure 7.5: UVa-E combustor: Time-evolution of the instantaneous solution at Station 2 when the 14-species reaction mechanism is used (cross-plane contours; first row: t=0 seconds, second row: t=0.00075 seconds, third row: t=0.0015 seconds, fourth row: t=0.00224 seconds; each column corresponds to a particular variable)
Figure 7.6: UVa-E combustor: Time-evolution of the instantaneous solution at Station 3 when the 14-species reaction mechanism is used (cross-plane contours; first row: t=0 seconds, second row: t=0.00075 seconds, third row: t=0.0015 seconds, fourth row: t=0.00224 seconds; each column corresponds to a particular variable)
Figure 7.7: UVA-E combustor: Time-evolution of the line-of-sight species temperature and column-densities when the 14-species reaction mechanism is used (lines: simulation results, circles: experimental data; data is time-averaged over successive sets of 20 frames and each line-plot corresponds to time-averaged data for a particular set of 20 frames)
7.6.2 TP-2 Reaction Mechanism

Instantaneous Centerplane Contours

Instantaneous centerplane contours of temperature, density-gradient, pressure, and Mach number are shown in Figure 7.8. The density-gradient contours show the overall shock structure and the flame shape inside the combustor and extender sections. The flame is clearly anchored to the leading edge of the cavity, and with downstream progression, the vertical extent of the flame is steadily increasing. From the temperature contours it is evident that, compared to the flame in the combustor section and the straight section of the extender, the flame is relatively cooler in the divergent section of the extender. A similar trend can be seen in the pressure contours, where the pressures in the divergent section of the extender are generally higher than the pressures in the upstream regions. The Mach number contours in Figure 7.8d show that, downstream of the leading edge of the cavity, the flow is supersonic in the freestream region and is subsonic inside the flame. While the flow velocities inside the flame are comparable to the freestream velocities, the low Mach numbers within the flame are a consequence of the high temperatures inside the flame.

Figure 7.9 shows centerplane contours of species mass-fractions (\( \text{C}_2\text{H}_4 \), \( \text{CO}_2 \), and \( \text{CO} \)) and equivalence ratio. For reference purposes, in Figure 7.9a, the locations of Stations 1, 2, and 3 are shown. From the \( \text{C}_2\text{H}_4 \) mass-fraction contours, it is evident that ethylene is non-existent within the cavity region. This means that all the ethylene entrained into the cavity is consumed in the combustion process. The presence of significant amounts of \( \text{CO} \) inside the cavity indicates that the combustion process is still incomplete. The upstream half of the cavity contains lower amounts of \( \text{CO} \) compared to the downstream half. Not surprisingly, the upstream half contains higher amounts of \( \text{CO}_2 \) compared to the downstream half. This could mean that the residence time of the fluid is higher in the upstream half of the cavity compared to the residence time in the downstream half, which basically gives the reacting mixture more time to progress towards the end stage of the combustion process.

With the entrainment of more fluid into the cavity, the still reacting fluid within the cavity is pushed out. Also, non-reacting fraction of ethylene that is not entrained into the cavity propagates downstream at the freestream velocity. Figures 7.9a and 7.9d show that, close to the wall, equivalence ratios at Station 3 and further downstream are nearly zero. Residual quantities of ethylene are present along the outer edges of the flame.
Figure 7.8: UVa-E combustor: Instantaneous centerplane contours of temperature, density-gradient, pressure, and Mach number with the TP-2 reaction mechanism
Downstream of Station 3, significant amounts of CO are present (Figure 7.9b) close to the wall, suggesting that the combustion process is still incomplete at this point. By the time the flow reaches the end of the straight section of the extender (Point A in Figure 7.9a), the combustion process reaches its final stages, which is evident from the near zero mass-fraction values of CO at point A. Downstream of this point, since there is no significant heat release due to combustion, the entrainment of the cooler freestream air into the flame decreases the flame temperatures, which is evident from Figure 7.8b.

**Time-Averaged Cross-Plane Contours**

Time-averaged cross-plane contours for temperature, species mass-fractions, and equivalence ratio are shown in Figures 7.10, 7.11, and 7.12. Temperature contours at Stations 1 and 2 indicate that the overall shape of the flame is asymmetric, which can be attributed to the asymmetry in the temperature profile at the inflow of the isolator. At Station 3, close to the wall, mass-fractions and equivalence ratios of ethylene are negligible. Further away from the wall, at Station 3, the equivalence ratios are low (around 0.1), suggesting that the fuel-consumption is close to completion, but not entirely complete. CO mass-fraction values are highest within the cavity at Station 1 and lowest at Station 3, which indicates that the combustion process is still in progress at Station 3 and that it is closer to completion at Station 3 than it is at Station 1.

**H₂O Temperature, Column-Density, and Mass-Fraction**

In Figure 7.13, time-averaged line-of-sight H₂O temperature, column-density, and mass-fraction profiles at all three stations are compared with the experiments. At Station 1, the predicted profiles for H₂O temperature and column-density agree well with the experiments, except, very close to the upper wall at Station 1, H₂O temperatures are over-predicted by around 200 K and the column-densities are minimally under-predicted. At Stations 2 and 3, H₂O temperatures are over-predicted; the peak values from the simulations and experiments are around 2100 K and 1600 K, respectively. The predicted H₂O column-density profiles show a good match with the experimental data at Stations 1 and 2. At Station 3, H₂O column-densities are consistently under-predicted throughout the range over which experimental data is available.

A comparison of experimental H₂O temperature profiles from Stations 1, 2, and 3 suggests that the peak flame temperatures are lower downstream compared to inside
Figure 7.9: UVa-E combustor: Instantaneous centerplane contours of mass-fractions of various species with the TP-2 reaction mechanism.
Figure 7.10: UVa-E combustor: Time-averaged cross-plane contours at Station 1 with the TP-2 reaction mechanism

Figure 7.11: UVa-E combustor: Time-averaged cross-plane contours at Station 2 with the TP-2 reaction mechanism

Figure 7.12: UVa-E combustor: Time-averaged cross-plane contours at Station 3 with the TP-2 reaction mechanism; ER: Equivalence Ratio; black line in Figure 7.10e is the contour line for ER = 1.0
the cavity. However, the experimental column-density profiles suggest that the overall production of H$_2$O increases further downstream, which means that the combustion process is still in progress. Combustion should increase the flame temperatures; however, the trend observed in the experimental measurements is the opposite. It is possible that the heat release due to combustion at Stations 2 and 3 is not as high as it is at Station 1. This decrease in the heat release coupled with the entrainment of higher amounts cooler air from the freestream can result in lower flame temperatures at Stations 2 and 3 compared to Station 1. However, the predicted H$_2$O temperature profiles suggest that the flame observed in the simulations has enough heat release at Stations 2 and 3 to keep the peak H$_2$O temperature values at 2100 K. Also, all the three predicted H$_2$O column-density profiles are consistent with the predicted H$_2$O temperature profiles. All three stations have nearly the same peak H$_2$O temperature and column-density values. Finally, at all three stations, the predicted H$_2$O mass-fraction profiles closely match with the experimental profiles, except for a minimal under-prediction at Station 3.

**CO Temperature and Column-Density**

Figure 7.14a compares the predicted time-averaged CO temperature and column-density profiles with the experimental measurements at Stations 1 and 2. At Station 1, the predicted and experimental peak values for CO temperature are nearly the same. In the predicted profile, the CO temperature values steadily increase with distance from the lower wall of the combustor. Close to the upper wall, the CO temperature values from the simulations steeply decrease, which is due to the isothermal boundary condition used in the simulations. While the overall trend observed in the experiments is similar, the initial increase in the measured CO temperature values is not steady. At Station 2, the predicted peak value of CO temperature is around 2100 K, whereas the measured peak value is 1750 K. Overall, the measured CO temperature values increase with the distance from the lower wall, but not as steadily as the measured H$_2$O temperature and predicted temperature values at Stations 1 and 2. At both these stations, the column-densities are over-predicted, with an over-prediction of around 100 percent at Station 1. The fact that the peak experimental values of CO column-densities at Stations 1 and 2 are nearly the same suggests that the oxidation process is still in progress at Station 2. However, the peak CO temperature at Station 2 is lower than the peak CO temperature at Station 1, which is the same trend followed by the measured H$_2$O temperature values. In all the
Figure 7.13: UVa-E combustor: H$_2$O temperature, column-density, and mass-fraction profiles at all three stations.
line-of-sight comparisons (Figures 7.13 and 7.14), the standard deviation at each point is also plotted.

![Graphs of CO temperature and column density](image)

(a) CO temperature

(b) CO column density

Figure 7.14: UVa-E combustor: CO temperature and column-density profiles at Stations 1 and 2

**CO$_2$ Column-Density**

Figure 7.15 shows the predicted and experimental CO$_2$ column-density profiles at Stations 1 and 2. At Station 1, except in the region very close to the upper wall inside the cavity, the predicted and experimental column-density profiles closely follow each other. At Station
2, while there is an under-prediction in the column-densities in the freestream, there is an over-prediction closer to the upper wall of the combustor. Except for the standard deviations in CO and CO$_2$ column-densities close to the upper wall of the combustor at Station 1, the standard deviations are very low for all other variables, which suggests that the flow is statistically very stable.

Figure 7.15: UVa-E combustor: CO$_2$ column-density profiles at Stations 1 and 2

**Pressure along the Upper Wall of the Combustor**

The pressure variation along the upper wall of the UVa-E combustor from simulation is compared with the experimental pressure profile in Figure 7.16. The standard deviations in the predicted pressure values are also shown in the same figure on a different axis. Upstream of the cavity leading edge ($x/H<0$), both profiles show a series of variations in pressure, which are very small in magnitude. However, the magnitudes of these variations are higher in the experiment compared to those from the simulation. Also, the standard deviations in the predicted pressure values are very small upstream of $x/H<0$. The magnitude and location of the pressure rise, which is due to the obstruction created by the flame, are very accurately predicted in the simulations. The simulation also accurately captures the variation of pressure downstream of the cavity leading edge. The accurate prediction of the pressure rise (location and magnitude) and the downstream variation of pressure suggests that the overall heat release and flame shape are accurately predicted.
in the simulations.

Figure 7.16: UVa-E combustor: Pressure variation along the upper wall; H=0.356 inches is the cavity depth; x/H=0 corresponds to the location of the leading edge of the cavity
Chapter 8

Summary and Conclusions

In the present study, reactive flows through different scramjet configurations were simulated using hybrid LES/RANS methods. The present study was focused on algorithmic and modeling sensitivity studies, formulation and testing of subgrid closures for modeling turbulence-chemistry interactions in a finite-rate chemistry large-eddy simulation framework, and LES of reactive flow through an ethylene fueled cavity flameholder. Also, throughout the present study, focus was on accounting for facility-dependent effects to as large an extent as feasible. The end result of this study is an enhanced version of NCSU’s hybrid LES/RANS solver REACTMB, which contains new modules developed for incorporating subgrid closures for filtered species production rates, a platform independent implementation of a modified version of the SEM of Jarrin et al. [65], a real-time visualization capability using LLNL’s VisIt visualization tool, and the new modules for reduced reaction mechanisms for ethylene-air kinetics.

The sensitivity study was mainly aimed at predicting an accurate flame-stabilization location for the DLR combustor. The effects of different modeling and algorithmic variations on the predictive capability of the solver were investigated comprehensively. These variations include: grid topologies, flux reconstruction methods, reaction mechanisms, a synthetic eddy method to aid mixing, and inflow boundary conditions. The study was performed by systematically making one variation at a time to narrow down the influence of the variation on the predicted solution. The end result of the study is a thorough understanding of the consequences of making a particular choice to model a physical phenomenon. The study showed that the choice of the reduced reaction mechanism used and the accurate representation of the facility-dependent effects using appropriate
boundary conditions have a significant influence on the predicted solution.

The influences of several subgrid closures (PaSR(0), PaSR(1), PaSR(SS), and SS), which account for the effect of turbulent-chemistry interactions on the species production rates, were also studied in detail. These subgrid closure models generally decrease the magnitude of the species production rates, relative to the ‘laminar chemistry’ closure. As test cases, reactive flows through the DLR combustor and the UVa-A combustor were considered. Both flows differ in terms of the type of fuel injection system used, flame shape, and internal flow pattern. Results show that the impact of the subgrid closures on the reactive flow through the DLR combustor is negligible. Except for PaSR(0), all other subgrid closures predict nearly identical results. Compared to the DLR combustor, the subgrid closures have a more pronounced influence on the predicted flow through the UVa-A combustor, and the temperature contours at different axial locations confirm this. Given the comprehensive experimental data set available for the reactive flow through the UVa-A combustor, the accuracy of the predictions by various subgrid closures is quantified using an error analysis procedure. Based on these errors, the performance of each model is assessed using a metric that compares a model’s accuracy with respect to a baseline model (Burke et al. ‘laminar chemistry’). This performance metric revealed that relative to the baseline model, Jachimowski ‘laminar chemistry’ and Burke et al. scale-similarity provide the most improvement, but the degree of improvement is quite modest.

Finally, reactive flow through an ethylene fueled cavity flameholder was simulated using two different reduced reaction mechanisms for modeling ethylene-air kinetics: 14- and 22-species reaction mechanisms. While the 14-species mechanism resulted in a flame blowout, predicted results using the 22-species mechanism showed excellent agreement with experimental data, especially, H$_2$O mole-fraction and wall pressure along the upper wall of the combustor. The predictions, in general, compare well with experimental data inside the cavity. However, experiments suggest that the flame temperatures further downstream are lower than the one predicted in the simulations.
REFERENCES


Appendix A

Reaction Mechanisms

Details of the various reaction mechanisms used in the present work are presented here. General notation used to describe particular reaction types is described below:

1. Reactions $R^0$ & $R^\infty$ essentially represent a single reaction, whose reaction rate is strongly dependent on pressure. The overall forward rate coefficient for this reaction is calculated by blending the rate coefficients of the $R^0$ and $R^\infty$ reactions, as described in §2.1.1. Values of constants required to perform this blending ($k_{f,0}, k_{f,\infty}, a, T^*, T^{**},$ and $T^{***}$) are given for the Ó Connaire [5] and Burke [6] reaction mechanisms.

2. Reactions $R^1$ & $R^2$ are duplicates of the same reaction, and they should be treated as two separate reactions with different rate coefficients.
A.1 Jachimowski Reaction Mechanism

Table A.1: Jachimowski reaction mechanism [2]

<table>
<thead>
<tr>
<th>Reaction #</th>
<th>Reaction</th>
<th>C</th>
<th>(\eta)</th>
<th>(E_a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\text{H}_2 + \text{O}_2 \rightleftharpoons \text{HO}_2 + \text{H})</td>
<td>(7.00 \times 10^{14})</td>
<td>0.0</td>
<td>(5.68 \times 10^4)</td>
</tr>
<tr>
<td>2</td>
<td>(\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O})</td>
<td>(2.20 \times 10^{14})</td>
<td>0.0</td>
<td>(1.68 \times 10^4)</td>
</tr>
<tr>
<td>3</td>
<td>(\text{O} + \text{H}_2 \rightleftharpoons \text{OH} + \text{H})</td>
<td>(5.06 \times 10^4)</td>
<td>2.67</td>
<td>(6.29 \times 10^3)</td>
</tr>
<tr>
<td>4</td>
<td>(\text{OH} + \text{H}_2 \rightleftharpoons \text{H}_2\text{O} + \text{H})</td>
<td>(2.16 \times 10^8)</td>
<td>1.51</td>
<td>(3.43 \times 10^3)</td>
</tr>
<tr>
<td>5</td>
<td>(\text{OH} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O})</td>
<td>(1.50 \times 10^9)</td>
<td>1.14</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>(\text{H} + \text{OH} + \text{M} \rightleftharpoons \text{H}_2\text{O} + \text{M})</td>
<td>(8.62 \times 10^{21})</td>
<td>-2.0</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>(\text{H} + \text{H} + \text{M} \rightleftharpoons \text{H}_2 + \text{M})</td>
<td>(7.30 \times 10^{17})</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>(\text{H} + \text{O} + \text{M} \rightleftharpoons \text{OH} + \text{M})</td>
<td>(2.60 \times 10^{16})</td>
<td>-0.6</td>
<td>0.0</td>
</tr>
<tr>
<td>9</td>
<td>(\text{O} + \text{O} + \text{M} \rightleftharpoons \text{O}_2 + \text{M})</td>
<td>(1.10 \times 10^{17})</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>(\text{H} + \text{O}_2 + \text{M} \rightleftharpoons \text{HO}_2 + \text{M})</td>
<td>(2.30 \times 10^{18})</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>11</td>
<td>(\text{HO}_2 + \text{H} \rightleftharpoons \text{OH} + \text{OH})</td>
<td>(1.50 \times 10^{14})</td>
<td>0.0</td>
<td>(1.0 \times 10^3)</td>
</tr>
<tr>
<td>12</td>
<td>(\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH})</td>
<td>(2.00 \times 10^{13})</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>13</td>
<td>(\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2)</td>
<td>(2.00 \times 10^{13})</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>14</td>
<td>(\text{HO}_2 + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2)</td>
<td>(2.00 \times 10^{12})</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>(\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2)</td>
<td>(1.70 \times 10^{12})</td>
<td>0.0</td>
<td>(3.78 \times 10^3)</td>
</tr>
<tr>
<td>16</td>
<td>(\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{OH} + \text{H}_2\text{O})</td>
<td>(1.00 \times 10^{13})</td>
<td>0.0</td>
<td>(3.58 \times 10^3)</td>
</tr>
<tr>
<td>17</td>
<td>(\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{OH} + \text{HO}_2)</td>
<td>(2.80 \times 10^{13})</td>
<td>0.0</td>
<td>(6.4 \times 10^3)</td>
</tr>
<tr>
<td>18</td>
<td>(\text{OH} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2)</td>
<td>(7.00 \times 10^{12})</td>
<td>0.0</td>
<td>(1.435 \times 10^3)</td>
</tr>
<tr>
<td>19</td>
<td>(\text{OH} + \text{OH} + \text{M} \rightleftharpoons \text{H}_2\text{O}_2 + \text{M})</td>
<td>(1.60 \times 10^{22})</td>
<td>-2.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table A.2: Jachimowski reaction mechanism: Chaperon efficiencies for various species

<table>
<thead>
<tr>
<th>Species</th>
<th>(TB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{H}_2)</td>
<td>2.5</td>
</tr>
<tr>
<td>(\text{H}_2\text{O})</td>
<td>16.0</td>
</tr>
<tr>
<td>all others</td>
<td>1.0</td>
</tr>
</tbody>
</table>
A.2 Seven-Species Reaction Mechanism

Table A.3: Seven-species, seven-step reaction mechanism [3, 4]

<table>
<thead>
<tr>
<th>Reaction #</th>
<th>Reaction</th>
<th>$C$</th>
<th>$\eta$</th>
<th>$E_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H + OH + M ⇌ H$_2$O + M</td>
<td>$0.221 \times 10^{23}$</td>
<td>-2.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>H + H + M ⇌ H$_2$ + M</td>
<td>$0.730 \times 10^{18}$</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>H$_2$ + O$_2$ ⇌ OH + OH</td>
<td>$0.170 \times 10^{14}$</td>
<td>0.0</td>
<td>24157.0</td>
</tr>
<tr>
<td>4</td>
<td>H + O$_2$ ⇌ OH + O</td>
<td>$0.120 \times 10^{14}$</td>
<td>-0.91</td>
<td>8310.5</td>
</tr>
<tr>
<td>5</td>
<td>OH + H$_2$ ⇌ H$_2$O + H</td>
<td>$0.220 \times 10^{14}$</td>
<td>0.0</td>
<td>2591.8</td>
</tr>
<tr>
<td>6</td>
<td>O + H$_2$ ⇌ OH + H</td>
<td>$0.506 \times 10^{5}$</td>
<td>2.67</td>
<td>3165.6</td>
</tr>
<tr>
<td>7</td>
<td>OH + OH ⇌ H$_2$O + O</td>
<td>$0.630 \times 10^{13}$</td>
<td>0.0</td>
<td>548.6</td>
</tr>
</tbody>
</table>

Table A.4: Seven-species, seven-step reaction mechanism: Chaperon efficiencies for various species

<table>
<thead>
<tr>
<th></th>
<th>N$_2$</th>
<th>O$_2$</th>
<th>H$_2$</th>
<th>H$_2$O</th>
<th>OH</th>
<th>O</th>
<th>H</th>
</tr>
</thead>
<tbody>
<tr>
<td>$TB$ (1)</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>16.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$TB$ (2)</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>16.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>
## A.3 Ó Connaire *et al.* Reaction Mechanism

Table A.5: Ó Connaire reaction mechanism [5]

<table>
<thead>
<tr>
<th>Reaction #</th>
<th>Reaction</th>
<th>$C$</th>
<th>$\eta$</th>
<th>$E_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H_2O + M \rightleftharpoons H + OH + M$</td>
<td>$1.912 \times 10^{24}$</td>
<td>-1.830</td>
<td>$1.185 \times 10^5$</td>
</tr>
<tr>
<td>2</td>
<td>$H_2 + M \rightleftharpoons H + H + M$</td>
<td>$4.577 \times 10^{19}$</td>
<td>-1.400</td>
<td>$1.0438 \times 10^5$</td>
</tr>
<tr>
<td>3</td>
<td>$H + O_2 + M \rightleftharpoons HO_2 + M$</td>
<td>$3.482 \times 10^{16}$</td>
<td>-0.411</td>
<td>$-1.1150 \times 10^3$</td>
</tr>
<tr>
<td>4</td>
<td>$H_2O_2 + M \rightleftharpoons 2OH + M$</td>
<td>$1.475 \times 10^{12}$</td>
<td>0.6</td>
<td>0.0000</td>
</tr>
<tr>
<td>5</td>
<td>$H_2O_2 \rightleftharpoons 2OH$</td>
<td>$1.202 \times 10^{17}$</td>
<td>0.0</td>
<td>45500.0</td>
</tr>
<tr>
<td>6</td>
<td>$OH + M \rightleftharpoons H + O + M$</td>
<td>$9.880 \times 10^{17}$</td>
<td>-0.74</td>
<td>$1.021 \times 10^5$</td>
</tr>
<tr>
<td>7</td>
<td>$O_2 + M \rightleftharpoons O + O + M$</td>
<td>$4.515 \times 10^{17}$</td>
<td>-0.64</td>
<td>$1.189 \times 10^5$</td>
</tr>
<tr>
<td>8</td>
<td>$H + O_2 \rightleftharpoons OH + O$</td>
<td>$1.915 \times 10^{14}$</td>
<td>0.0</td>
<td>$1.644 \times 10^4$</td>
</tr>
<tr>
<td>9</td>
<td>$OH + H_2 \rightleftharpoons H_2O + H$</td>
<td>$0.216 \times 10^9$</td>
<td>1.51</td>
<td>$0.343 \times 10^4$</td>
</tr>
<tr>
<td>10</td>
<td>$O + H_2 \rightleftharpoons OH + H$</td>
<td>$0.508 \times 10^5$</td>
<td>2.67</td>
<td>$0.629 \times 10^4$</td>
</tr>
<tr>
<td>11</td>
<td>$H_2O + O \rightleftharpoons OH + OH$</td>
<td>$2.97 \times 10^6$</td>
<td>2.02</td>
<td>$1.34 \times 10^4$</td>
</tr>
<tr>
<td>12</td>
<td>$HO_2 + H \rightleftharpoons OH + OH$</td>
<td>$2.89 \times 10^{13}$</td>
<td>0.0</td>
<td>$-4.970 \times 10^2$</td>
</tr>
<tr>
<td>13</td>
<td>$HO_2 + O \rightleftharpoons OH + O_2$</td>
<td>$7.079 \times 10^{13}$</td>
<td>0.0</td>
<td>$2.95 \times 10^2$</td>
</tr>
<tr>
<td>14</td>
<td>$H_2O + O \rightleftharpoons OH + O_2$</td>
<td>$0.325 \times 10^{14}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>$H_2O_2 + O \rightleftharpoons HO_2 + HO_2$</td>
<td>$4.634 \times 10^{16}$</td>
<td>-0.35</td>
<td>$5.067 \times 10^4$</td>
</tr>
<tr>
<td>16</td>
<td>$H_2O_2 + O \rightleftharpoons HO_2 + HO_2$</td>
<td>$1.434 \times 10^{13}$</td>
<td>-0.35</td>
<td>$3.706 \times 10^4$</td>
</tr>
<tr>
<td>17</td>
<td>$H_2O_2 + H \rightleftharpoons HO_2 + H_2$</td>
<td>$6.025 \times 10^{13}$</td>
<td>0.0</td>
<td>$0.795 \times 10^4$</td>
</tr>
<tr>
<td>18</td>
<td>$H_2O_2 + OH \rightleftharpoons HO_2 + H_2$</td>
<td>$1.00 \times 10^{12}$</td>
<td>0.0</td>
<td>0.0000</td>
</tr>
<tr>
<td>19</td>
<td>$H_2O_2 + OH \rightleftharpoons HO_2 + H_2$</td>
<td>$5.80 \times 10^{14}$</td>
<td>0.0</td>
<td>$9.557 \times 10^3$</td>
</tr>
<tr>
<td>20</td>
<td>$H_2O_2 + OH \rightleftharpoons HO_2 + H_2$</td>
<td>$0.241 \times 10^{14}$</td>
<td>0.0</td>
<td>$0.397 \times 10^4$</td>
</tr>
<tr>
<td>21</td>
<td>$H_2O_2 + O \rightleftharpoons OH + HO_2$</td>
<td>$9.550 \times 10^6$</td>
<td>2.0</td>
<td>$3.970 \times 10^3$</td>
</tr>
<tr>
<td>22</td>
<td>$HO_2 + H \rightleftharpoons H_2 + O_2$</td>
<td>$1.66 \times 10^{13}$</td>
<td>0.0</td>
<td>$0.823 \times 10^3$</td>
</tr>
</tbody>
</table>
Table A.6: Ó Connaire reaction mechanism: Chaperon efficiencies for various species

<table>
<thead>
<tr>
<th></th>
<th>N$_2$</th>
<th>O$_2$</th>
<th>H$_2$</th>
<th>H$_2$O</th>
<th>OH</th>
<th>O</th>
<th>H</th>
<th>HO$_2$</th>
<th>H$_2$O$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TB (1)</td>
<td>1.0</td>
<td>1.0</td>
<td>0.73</td>
<td>12.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>TB (2)</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>TB (3$^0$)</td>
<td>1.0</td>
<td>1.0</td>
<td>1.3</td>
<td>14.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>TB (4$^0$)</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>TB (5)</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>TB (6)</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table A.7: Troe coefficients for the Ó Connaire reaction mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$a$</th>
<th>$T^{***}$</th>
<th>$T^*$</th>
<th>$T^{**}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.5</td>
<td>$1 \times 10^{-30}$</td>
<td>$1 \times 10^{30}$</td>
<td>$1 \times 10^{30}$</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>$1 \times 10^{-30}$</td>
<td>$1 \times 10^{30}$</td>
<td>$1 \times 10^{30}$</td>
</tr>
</tbody>
</table>
## A.4 Burke et al. Reaction Mechanism

Table A.8: Burke reaction mechanism [6]

<table>
<thead>
<tr>
<th>Reaction #</th>
<th>Reaction</th>
<th>C</th>
<th>η</th>
<th>E_a</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H + O₂ ⇌ O + OH</td>
<td>1.04 × 10^{14}</td>
<td>0.0</td>
<td>1.531 × 10^{4}</td>
</tr>
<tr>
<td>2₁</td>
<td>O + H₂ ⇌ H + OH</td>
<td>3.820 × 10^{12}</td>
<td>0.0</td>
<td>7.948 × 10^{3}</td>
</tr>
<tr>
<td>2²</td>
<td>O + H₂ ⇌ H + OH</td>
<td>8.79 × 10^{14}</td>
<td>0.0</td>
<td>1.917 × 10^{4}</td>
</tr>
<tr>
<td>3</td>
<td>H₂ + OH ⇌ H₂O + H</td>
<td>2.160 × 10^{8}</td>
<td>1.51</td>
<td>3.430 × 10^{3}</td>
</tr>
<tr>
<td>4</td>
<td>OH + OH ⇌ O + H₂O</td>
<td>3.34 × 10^{4}</td>
<td>2.42</td>
<td>1.930 × 10^{3}</td>
</tr>
<tr>
<td>5</td>
<td>H₂ + M ⇌ H + H + M</td>
<td>4.58 × 10^{19}</td>
<td>1.40</td>
<td>1.040 × 10^{5}</td>
</tr>
<tr>
<td>6</td>
<td>O + O + M ⇌ O₂ + M</td>
<td>6.16 × 10^{15}</td>
<td>0.50</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>O + H + M ⇌ OH + M</td>
<td>4.71 × 10^{18}</td>
<td>1.00</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>H₂O + M ⇌ H + OH + M</td>
<td>6.06 × 10^{27}</td>
<td>3.32</td>
<td>1.208 × 10^{5}</td>
</tr>
<tr>
<td>9₀</td>
<td>H + O₂ + M ⇌ HO₂ + M</td>
<td>6.37 × 10^{20}</td>
<td>1.72</td>
<td>5.25 × 10^{2}</td>
</tr>
<tr>
<td>9∞</td>
<td>H + O₂ ⇌ HO₂</td>
<td>4.65 × 10^{12}</td>
<td>0.44</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>O₂ + H ⇌ H₂ + O₂</td>
<td>2.75 × 10^{6}</td>
<td>2.09</td>
<td>1.451 × 10^{3}</td>
</tr>
<tr>
<td>11</td>
<td>O₂ + H ⇌ OH + OH</td>
<td>7.08 × 10^{13}</td>
<td>0.0</td>
<td>2.950 × 10^{2}</td>
</tr>
<tr>
<td>12</td>
<td>O₂ + O ⇌ O₂ + OH</td>
<td>2.85 × 10^{10}</td>
<td>1.00</td>
<td>7.239 × 10^{2}</td>
</tr>
<tr>
<td>13</td>
<td>O₂ + OH ⇌ H₂O + O₂</td>
<td>2.89 × 10^{13}</td>
<td>0.0</td>
<td>4.970 × 10^{2}</td>
</tr>
<tr>
<td>14₁</td>
<td>O₂ + HO₂ ⇌ H₂O₂ + O₂</td>
<td>4.20 × 10^{14}</td>
<td>0.0</td>
<td>1.200 × 10^{4}</td>
</tr>
<tr>
<td>14²</td>
<td>O₂ + HO₂ ⇌ H₂O₂ + O₂</td>
<td>1.30 × 10^{11}</td>
<td>0.0</td>
<td>1.630 × 10^{3}</td>
</tr>
<tr>
<td>15₀</td>
<td>H₂O₂ + M ⇌ OH + OH + M</td>
<td>2.49 × 10^{24}</td>
<td>2.30</td>
<td>4.875 × 10^{4}</td>
</tr>
<tr>
<td>15∞</td>
<td>H₂O₂ ⇌ OH + OH</td>
<td>2.00 × 10^{12}</td>
<td>0.90</td>
<td>4.875 × 10^{4}</td>
</tr>
<tr>
<td>16</td>
<td>H₂O₂ + H ⇌ H₂O + OH</td>
<td>2.41 × 10^{13}</td>
<td>0.0</td>
<td>3.970 × 10^{3}</td>
</tr>
<tr>
<td>17</td>
<td>H₂O₂ + H ⇌ HO₂ + H₂</td>
<td>4.82 × 10^{13}</td>
<td>0.0</td>
<td>7.95 × 10^{3}</td>
</tr>
<tr>
<td>18</td>
<td>H₂O₂ + O ⇌ OH + HO₂</td>
<td>9.55 × 10^{6}</td>
<td>2.00</td>
<td>3.970 × 10^{3}</td>
</tr>
<tr>
<td>19₁</td>
<td>H₂O₂ + OH ⇌ HO₂ + H₂O</td>
<td>1.74 × 10^{12}</td>
<td>0.0</td>
<td>3.180 × 10^{2}</td>
</tr>
<tr>
<td>19²</td>
<td>H₂O₂ + OH ⇌ HO₂ + H₂O</td>
<td>7.59 × 10^{13}</td>
<td>0.0</td>
<td>7.270 × 10^{3}</td>
</tr>
</tbody>
</table>
Table A.9: Burke reaction mechanism: Chaperon efficiencies for various species

<table>
<thead>
<tr>
<th>TB (5)</th>
<th>TB (6)</th>
<th>TB (7)</th>
<th>TB (8)</th>
<th>TB (9)</th>
<th>TB (15)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>$O_2$</td>
<td>$H_2$</td>
<td>$H_2O$</td>
<td>$H_2O_2$</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>1.5</td>
<td>3.0</td>
<td>0.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>0.78</td>
<td>2.0</td>
<td>14.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>1.2</td>
<td>3.7</td>
<td>7.5</td>
<td>7.7</td>
<td></td>
</tr>
</tbody>
</table>

Table A.10: Troe coefficients for the Burke reaction mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$a$</th>
<th>$T^*$</th>
<th>$T^{**}$</th>
<th>$T^{***}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>0.5</td>
<td>$1.0 \times 10^{30}$</td>
<td>0.0</td>
<td>$1.0 \times 10^{30}$</td>
</tr>
<tr>
<td>15</td>
<td>0.42</td>
<td>$1.0 \times 10^{30}$</td>
<td>0.0</td>
<td>$1.0 \times 10^{30}$</td>
</tr>
</tbody>
</table>
### A.5 Modified Gokulakrishnan et al. Reaction Mechanism

Table A.11: Modified version of the Gokulakrishnan et al. reaction mechanism [7]

<table>
<thead>
<tr>
<th>Reaction #</th>
<th>Reaction</th>
<th>$C_r$</th>
<th>$\eta$</th>
<th>$E_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H + OH + M $\rightleftharpoons$ H$_2$O + M</td>
<td>3.8 x 10$^{14}$</td>
<td>-2.0</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>H$_2$ + M $\rightleftharpoons$ 2H + M</td>
<td>4.55 x 10$^{19}$</td>
<td>-1.4</td>
<td>1.0438 x 10$^5$</td>
</tr>
<tr>
<td>3$^0$</td>
<td>H + O$_2$ + M $\rightleftharpoons$ HO$_2$ + M</td>
<td>6.366 x 10$^{20}$</td>
<td>-1.72</td>
<td>5.248 x 10$^2$</td>
</tr>
<tr>
<td>3$^\infty$</td>
<td>H + O$_2$ $\rightleftharpoons$ HO$_2$</td>
<td>1.575 x 10$^{12}$</td>
<td>0.6</td>
<td>0.000</td>
</tr>
<tr>
<td>4$^0$</td>
<td>H$_2$O$_2$ + M $\rightleftharpoons$ 2OH + M</td>
<td>1.202 x 10$^{17}$</td>
<td>0.0</td>
<td>4.55 x 10$^4$</td>
</tr>
<tr>
<td>4$^\infty$</td>
<td>H$_2$O$_2$ $\rightleftharpoons$ 2OH</td>
<td>2.95 x 10$^{14}$</td>
<td>0.0</td>
<td>4.843 x 10$^4$</td>
</tr>
<tr>
<td>5</td>
<td>H + O + M $\rightleftharpoons$ OH + M</td>
<td>4.714 x 10$^{18}$</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>O + O + M $\rightleftharpoons$ O$_2$ + M</td>
<td>6.165 x 10$^{15}$</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>7$^0$</td>
<td>CO + O + M $\rightleftharpoons$ CO$_2$ + M</td>
<td>1.55 x 10$^{24}$</td>
<td>-2.79</td>
<td>4191</td>
</tr>
<tr>
<td>7$^\infty$</td>
<td>CO + O $\rightleftharpoons$ CO$_2$</td>
<td>1.80 x 10$^{10}$</td>
<td>0.0</td>
<td>2384</td>
</tr>
<tr>
<td>8</td>
<td>HCO + M $\rightleftharpoons$ H + CO + M</td>
<td>4.7485 x 10$^{11}$</td>
<td>0.659</td>
<td>14874</td>
</tr>
<tr>
<td>9</td>
<td>CH$_2$O + M $\rightleftharpoons$ HCO + H + M</td>
<td>3.30 x 10$^{39}$</td>
<td>-6.30</td>
<td>99900</td>
</tr>
<tr>
<td>10</td>
<td>CH$_2$O + M $\rightleftharpoons$ CO + H$_2$ + M</td>
<td>3.10 x 10$^{45}$</td>
<td>-8.0</td>
<td>97510</td>
</tr>
<tr>
<td>11</td>
<td>H + O$_2$ $\rightleftharpoons$ OH + O</td>
<td>3.547 x 10$^{15}$</td>
<td>-0.406</td>
<td>16599</td>
</tr>
<tr>
<td>12</td>
<td>OH + H$_2$ + H$_2$O + H</td>
<td>0.216 x 10$^{15}$</td>
<td>1.51</td>
<td>3430</td>
</tr>
<tr>
<td>13</td>
<td>O + H$_2$ $\rightleftharpoons$ OH + H</td>
<td>0.508 x 10$^{15}$</td>
<td>2.67</td>
<td>6290</td>
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<tr>
<td>14</td>
<td>H$_2$O + O $\rightleftharpoons$ OH + OH</td>
<td>2.97 x 10$^{6}$</td>
<td>2.02</td>
<td>13400</td>
</tr>
<tr>
<td>15</td>
<td>HO$_2$ + OH $\rightleftharpoons$ H$_2$ + O$_2$</td>
<td>2.39 x 10$^{13}$</td>
<td>0.0</td>
<td>-497</td>
</tr>
<tr>
<td>16</td>
<td>HO$_2$ + H $\rightleftharpoons$ OH + OH</td>
<td>7.079 x 10$^{13}$</td>
<td>0.0</td>
<td>295.</td>
</tr>
<tr>
<td>17</td>
<td>HO$_2$ + O $\rightleftharpoons$ OH + O$_2$</td>
<td>0.325 x 10$^{44}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>18$^4$</td>
<td>HO$_2$ + HO$_2$ $\rightleftharpoons$ H$_2$O$_2$ + O$_2$</td>
<td>4.20 x 10$^{14}$</td>
<td>0.0</td>
<td>11982</td>
</tr>
<tr>
<td>18$^5$</td>
<td>HO$_2$ + HO$_2$ $\rightleftharpoons$ H$_2$O$_2$ + O$_2$</td>
<td>1.30 x 10$^{14}$</td>
<td>0.0</td>
<td>-1.6294 x 10$^4$</td>
</tr>
<tr>
<td>19</td>
<td>H$_2$O$_2$ + H $\rightleftharpoons$ HO$_2$ + H$_2$</td>
<td>0.482 x 10$^{14}$</td>
<td>0.0</td>
<td>7950</td>
</tr>
<tr>
<td>20$^4$</td>
<td>H$_2$O$_2$ + OH + H$_2$O</td>
<td>1.00 x 10$^{12}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>20$^5$</td>
<td>H$_2$O$_2$ + OH $\rightleftharpoons$ H$_2$O + H$_2$O</td>
<td>5.80 x 10$^{14}$</td>
<td>0.0</td>
<td>9.557 x 10$^3$</td>
</tr>
<tr>
<td>21</td>
<td>H$_2$O$_2$ + H $\rightleftharpoons$ OH + H$_2$O</td>
<td>0.241 x 10$^{14}$</td>
<td>0.0</td>
<td>3970</td>
</tr>
<tr>
<td>22</td>
<td>H$_2$O$_2$ + O $\rightleftharpoons$ OH + HO$_2$</td>
<td>9.55 x 10$^{6}$</td>
<td>2.0</td>
<td>3970</td>
</tr>
<tr>
<td>23</td>
<td>HO$_2$ + H $\rightleftharpoons$ H$_2$ + O$_2$</td>
<td>1.66 x 10$^{13}$</td>
<td>0.0</td>
<td>823.</td>
</tr>
<tr>
<td>24</td>
<td>C$_2$H$_4$ + O$_2$ $\rightleftharpoons$ 2CH$_2$O</td>
<td>5.50 x 10$^{8}$</td>
<td>2.733</td>
<td>31106.55</td>
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<tr>
<td>25</td>
<td>CO + O$_2$ $\rightleftharpoons$ CO$_2$ + O</td>
<td>0.253 x 10$^{13}$</td>
<td>0.0</td>
<td>47700</td>
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<td>26</td>
<td>CO + HO$_2$ $\rightleftharpoons$ CO$_2$ + OH</td>
<td>3.01 x 10$^{15}$</td>
<td>0.0</td>
<td>230000</td>
</tr>
<tr>
<td>27</td>
<td>CO + OH $\rightleftharpoons$ CO$_2$ + H</td>
<td>2.229 x 10$^{15}$</td>
<td>1.89</td>
<td>-1158.7</td>
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<tr>
<td>28</td>
<td>HCO + O$_2$ $\rightleftharpoons$ CO + HO$_2$</td>
<td>0.758 x 10$^{13}$</td>
<td>0.0</td>
<td>410.</td>
</tr>
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<td>29</td>
<td>HCO + H $\rightleftharpoons$ CO + H$_2$</td>
<td>0.723 x 10$^{14}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>30</td>
<td>HCO + O $\rightleftharpoons$ CO + OH</td>
<td>0.302 x 10$^{14}$</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>31</td>
<td>HCO + OH $\rightleftharpoons$ CO + H$_2$O</td>
<td>0.302 x 10$^{14}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>32</td>
<td>HCO + O$_2$ $\rightleftharpoons$ CO + O$_2$ + H</td>
<td>3.00 x 10$^{15}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>33</td>
<td>HCO + HO$_2$ $\rightleftharpoons$ CO + OH + H</td>
<td>3.00 x 10$^{15}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>34</td>
<td>HCO + HCO $\rightleftharpoons$ H$_2$ + CO + CO</td>
<td>3.00 x 10$^{12}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>35</td>
<td>HCO + HCO $\rightleftharpoons$ CH$_2$O + CO</td>
<td>3.00 x 10$^{13}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>36</td>
<td>CH$_2$O + H $\rightleftharpoons$ HCO + H$_2$</td>
<td>5.74 x 10$^{10}$</td>
<td>1.9</td>
<td>27486.6</td>
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<tr>
<td>37</td>
<td>CH$_2$O + O $\rightleftharpoons$ HCO + OH</td>
<td>1.81 x 10$^{13}$</td>
<td>0.0</td>
<td>3080.</td>
</tr>
<tr>
<td>38</td>
<td>CH$_2$O + OH $\rightleftharpoons$ HCO + H$_2$O</td>
<td>3.43 x 10$^{9}$</td>
<td>1.18</td>
<td>-447</td>
</tr>
<tr>
<td>39</td>
<td>CH$_2$O + O$_2$ $\rightleftharpoons$ HCO + HO$_2$</td>
<td>1.24 x 10$^{8}$</td>
<td>3.0</td>
<td>52000.</td>
</tr>
<tr>
<td>40</td>
<td>CH$_2$O + HO$_2$ $\rightleftharpoons$ HCO + H$_2$O$_2$</td>
<td>4.11 x 10$^{4}$</td>
<td>2.50</td>
<td>10210</td>
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</table>

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Table A.12: Troe coefficients for the modified Gokulakrishnan reaction mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$a$</th>
<th>$T^*$</th>
<th>$T^{**}$</th>
<th>$T^{***}$</th>
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</thead>
<tbody>
<tr>
<td>3</td>
<td>0.8</td>
<td>$1.0 \times 10^{-30}$</td>
<td>$1.0 \times 10^{30}$</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>$1.0 \times 10^{-30}$</td>
<td>$1.0 \times 10^{30}$</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>0.5</td>
<td>$1.0 \times 10^{-30}$</td>
<td>$1.0 \times 10^{30}$</td>
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</tr>
</tbody>
</table>

Table A.13: Modified Gokulakrishnan reaction mechanism: Chaperon efficiencies for various species

<table>
<thead>
<tr>
<th></th>
<th>$O_2$</th>
<th>$H_2$</th>
<th>$H_2O$</th>
<th>$CO$</th>
<th>$CO_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$TB$ (1)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (2)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (3)</td>
<td>0.78</td>
<td>2.0</td>
<td>11.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (4)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (5)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (6)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (7)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (8)</td>
<td>1.0</td>
<td>2.5</td>
<td>6.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (9)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>$TB$ (10)</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.9</td>
<td>3.8</td>
</tr>
</tbody>
</table>
Appendix B

Reference Values for Sutherland’s Law

Table B.1: Sutherland’s law reference values (Table 1)

<table>
<thead>
<tr>
<th></th>
<th>N₂</th>
<th>O₂</th>
<th>H₂</th>
<th>H₂O</th>
<th>OH</th>
<th>O</th>
<th>H</th>
<th>HO₂</th>
<th>H₂O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>µ&lt;sub&gt;ref&lt;/sub&gt;</td>
<td>0.1663</td>
<td>0.1919</td>
<td>0.0841</td>
<td>0.1703</td>
<td>0.1826</td>
<td>0.1743</td>
<td>0.0701</td>
<td>0.1919</td>
<td>0.1919</td>
</tr>
<tr>
<td>S&lt;sub&gt;µ&lt;/sub&gt;</td>
<td>106.4</td>
<td>138.9</td>
<td>96.67</td>
<td>860.8</td>
<td>138.6</td>
<td>157.0</td>
<td>117.7</td>
<td>138.9</td>
<td>138.9</td>
</tr>
<tr>
<td>T&lt;sub&gt;µ&lt;/sub&gt;</td>
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<td>273.1</td>
<td>273.1</td>
<td>416.5</td>
<td>273.1</td>
<td>273.1</td>
<td>273.1</td>
<td>273.1</td>
<td>273.1</td>
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Table B.2: Sutherland’s law reference values (Table 2)

<table>
<thead>
<tr>
<th></th>
<th>C₂H₄</th>
<th>CH₂O</th>
<th>CO</th>
<th>CO₂</th>
<th>CH₃</th>
<th>CH₂CO</th>
<th>CH₃CHO</th>
<th>CH₄</th>
<th>C₂H₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>µ&lt;sub&gt;ref&lt;/sub&gt;</td>
<td>0.0960</td>
<td>0.4505</td>
<td>0.1657</td>
<td>0.1370</td>
<td>0.2104</td>
<td>0.3873</td>
<td>0.3873</td>
<td>0.3622</td>
<td>0.3667</td>
</tr>
<tr>
<td>S&lt;sub&gt;µ&lt;/sub&gt;</td>
<td>226.11</td>
<td>1089.25</td>
<td>136.11</td>
<td>222.22</td>
<td>1223.00</td>
<td>404.24</td>
<td>404.24</td>
<td>213.06</td>
<td>281.6</td>
</tr>
<tr>
<td>T&lt;sub&gt;µ&lt;/sub&gt;</td>
<td>273.11</td>
<td>1500.0</td>
<td>273.11</td>
<td>273.11</td>
<td>1500.0</td>
<td>1500.0</td>
<td>1500.0</td>
<td>1500.0</td>
<td>1500.0</td>
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Table B.3: Sutherland’s law reference values (Table 3)

<table>
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<tr>
<th></th>
<th>$\text{C}_2\text{H}_6$</th>
<th>$\text{C}_3\text{H}_6$</th>
<th>$\text{aC}_3\text{H}_5$</th>
<th>$\text{HCCO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_{ref}$</td>
<td>0.3394</td>
<td>0.3313</td>
<td>0.3313</td>
<td>0.3873</td>
</tr>
<tr>
<td>$S_\mu$</td>
<td>305.50</td>
<td>345.70</td>
<td>345.70</td>
<td>404.24</td>
</tr>
<tr>
<td>$T_\mu$</td>
<td>1500.0</td>
<td>1500.0</td>
<td>1500.0</td>
<td>1500.0</td>
</tr>
</tbody>
</table>
Appendix C

Integration of VisIt into REACTMB

To avoid transferring large data files from remote systems to local machines for monitoring the evolution of the numerical solution, Lawrence Livermore National Laboratory’s VisIt (https://wci.llnl.gov/codes/visit/about.html) visualization tool has been integrated into NCSU’s REACTMB. The integration is done in the following way:

1. Installation of VisIt using precompiled binaries in the home directory of the user.

2. Installation of the SILO libraries (https://wci.llnl.gov/codes/silo/) and executables in the home directory of the user.

3. Writing out individual block data files in PDB format using SILO Fortran interface. These data files are written into the ‘visit_silo/blockwise’ folder. This is done using the subroutine ‘blockwise_node()’.

4. Linking together all the block data files by writing out a master file, located in the ‘visit_silo/masterfile’ folder, using SILO Fortran interface. This is done using the subroutine ‘write_master()’.

5. Running a shell script ‘visit_silo/visit_script’, which in turn runs a Python script ‘visit_silo/contour_* .py’ through VisIt. This Python script can be manipulated to generate images with contours, isosurfaces, streamlines, lineplots, among others. Images are generated based on the variable name, and all the images generated in a particular dump have a time stamp in the name. VisIt automatically updates the time stamp based on the time stamps of the existing dumps of images. The images are placed in the folder ‘visit_silo/instant_images’.
6. The frequency at which these images are generated can be controlled using a file ‘itvisit’ located in the ‘visit_silo/visit_silo’ folder, which is located in the run directory. Apart from solution monitoring, VisIt can be used to generate publication quality plots and images. VisIt provides extensive control over the formatting of various elements that appear in the plots: legends, axis labels, ticks marks, color maps, 3-dimensional view points, among others.

The VisIt Python interface manual can be downloaded from:

The SILO interface manual can be downloaded from: