PATTON, CONRAD H. Turbulent Combustion Closure Modeling for High Speed LES. (Under the direction of Jack Edwards and Tarek Echekki.)

This work develops improved models that account for the effects of unresolved turbulent fluctuations on the chemical production terms in large-eddy simulation (LES) of high speed turbulent combustion. One application of these simulations is scramjet/ramjet combustion. Scramjet combustion is affected by the interplay between high turbulence levels, combustion kinetics, general compressibility effects, and convective time scales that are comparable to chemical time scales. There are also highly transient events occurring throughout the flowpath including moving shock waves, ignition and extinction events, and blowout or re-ignition events. Due to all of these complex physical phenomenon, finite-rate treatment of the chemical kinetics may be most appropriate. However, combustion chemistry occurs at the molecular levels and is affected strongly by reactant inhomogeneity. This means that fluctuations in temperature or species composition that are not being resolved by the scale of the LES simulations will have an effect on the chemical production terms. Therefore, the chemical production rates are affected by the interactions between the resolved eddies as well as the interactions of the unresolved (subgrid) eddies.

Acceptable results can be obtained using the 'laminar chemistry' assumption in certain cases; this is the evaluation of chemical production rates using filtered mean data. The trend is that 'laminar chemistry' (LC) generally over-estimates reactivity. This leads to flame temperatures that are higher than typically measured using non-intrusive diagnostics. Several relatively simple closures (e.g. partially-stirred reactor (PaSR), thickened-flame, scale-similarity, and flame wrinkling models) are available. However, most of these tend to diminish reactivity, and it is not clear that the effect of the unresolved fluctuations is to always reduce apparent reactivity. There are also advanced subgrid models that can handle finite-rate chemistry, but these are expensive. It is the goal of this research to determine candidate models of the type $\bar{\omega}_s(q) = f(q, \delta, ...) \omega_s(\bar{q})$ (similar to PaSR and thickened-flame methods), where $f$ is the 'enhancement factor.' The enhancement factor is designed to account for the effects of unresolved fluctuations on the apparent reactivity at the given mesh scale.

To progress towards a model form for the enhancement factor, a modified a priori analysis is developed that utilizes simultaneous mesh-sequenced large-eddy simulations of a reactive turbulent shear layer. These simulations are used to assess the errors associated with the unresolved fluctuations on the chemical production terms that result from coarsening the grid. In order to compare chemical source terms in a meaningful manner between grid levels, velocity coupling is used to ensure that eddy evolution is highly correlated between grid levels. This means that the largest eddies resolved on the coarse grid would match the corresponding eddies on the fine grid. Any differences observed between grid levels is assumed to be dominated by the effect of unresolved subgrid effects on the filtered chemical
production terms.

Based on the modified a priori analysis, a new family of combustion closure models is developed based on least-squares minimization (LSM) between the filtered fine-mesh chemical source terms and the chemical source terms on the coarse grid using laminar chemistry. Since fine-mesh information is not usually available, the filtered fine-mesh source term requires closure to implement the model. Several methods to accomplish this are proposed in this work. The first is a LSM-FS (filtered sources) model which uses test-filtered coarse grid chemical source terms. Heat release information can also be incorporated based on the test filtered chemical source terms as well (LSM-FS-H). An extension of these models is the LSM-MMD model which uses a min-mod operator to ensure the model will only attenuate reactivity. Scale-similarity and ‘optimal single point’ options are developed as well.

After identifying candidate model forms, select models are chosen for further testing in simulations for which experimental data is available for consideration. The first two test cases correspond to experiments conducted at the University of Virginia (UVa) for a hydrogen-fueled scramjet combustor. The third test case corresponds to another experiment conducted at UVa for an ethylene-fueled combustor. The simulation results using the selected models are compared with previous LES/RANS simulations using the laminar chemistry assumption and with some of the available experimental data. A fourth test case, the Volvo Validation Rig, is used to examine the models’ performance for a low-speed premixed flame. For this case, premixed propane-air mixture passes over a bluff body which creates a recirculation zone of hot products to provide a source of ignition for the incoming reactants. Velocity (both mean and fluctuations) and temperature profiles are compared at transverse and axial stations within the region of the flame.

Across all cases, the new family of closure models developed provided a consistent improvement in simulation predictions, relative to laminar chemistry, when compared with experimental data. The LSM-FS model was tested for all cases and was found to enhance reactivity in high strain regions and attenuate reactivity in well-mixed regions. Five different models were tested for the UVa hydrogen fueled combustor case. Adding a dependency on heat release to the LSM-FS model resulted in more enhancement in the high-strain regions, but did not result in significant change in the time-averaged results. The scale-similarity and LSM-JMPANN (optimal point model built using machine learning) models decreased reactivity the most with the smallest enhancement factor values. This resulted in more noticeable change in temperatures in the ignition region of the flame. The scale-similarity model also attenuated reactivity over the largest area of the flame followed by the LSM-MMD model. For the Volvo case, the models tested resulted in a reduction in reaction rate per unit flame area. This decreased the turbulent flame speeds and resulted in smaller fluctuations, which resulted in temperature and velocity fluctuation predictions that were closer to the experimental results, compared with laminar chemistry.
Turbulent Combustion Closure Modeling for High Speed LES

by
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A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Doctor of Philosophy

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DEDICATION

To my parents.
BIOGRAPHY

Conrad Patton was born on April 30, 1991 in Atlanta, Georgia to Frank and Tina Patton. His family moved to North Carolina around 1997, eventually moving to a small town called Blanch. Nearing graduation from Bartlett Yancey High School, Conrad applied to the Engineering school at North Carolina State University due to his excelling at math and science. While at NC State, Conrad decided to matriculate into Aerospace Engineering. Upon graduating with a Bachelors, Conrad was accepted to the Graduate school at NC State. Conrad was approached by Dr Hassan to discuss research opportunities in the CFD lab and subsequently met with Dr Edwards. Conrad was hired as a research assistant, initially pursuing a Master’s degree. Shortly after starting graduate school, Conrad was convinced to enroll in the direct path to Ph.D. program by his primary advisor, Dr Edwards. During his graduate studies Conrad worked under advisement of Dr Edwards in combustion closure modeling as well as numerous other reactive flow simulations using both RANS and hybrid LES/RANS techniques. Conrad plans to complete his studies by May 2017.
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## LIST OF SYMBOLS

### Roman Letters

- $a$: sound speed
- $c_p$: heat capacity
- $d$: distance
- $D_a$: Damköhler number
- $e$: specific internal energy
- $f$: enhancement factor
- $h$: specific enthalpy
- $k$: turbulent kinetic energy
- $L$: length scale
- $M$: Mach number
- $Pr$: Prandtl number
- $q$: heat release or generic flow variable
- $R$: gas constant
- $Re$: Reynolds number
- $Sc$: Schmidt number
- $t$: time
- $T$: temperature
- $u_i$: velocity vector
- $U$: bulk velocity
- $V_{s,i}$: species diffusion velocity
- $M_{w,s}$: species molecular weight
- $X_s$: species mole fraction
- $Y_s$: species mass fraction
- $x, y, z$: coordinate variables
- $Z$: mixture fraction

### Greek Letters

- $\alpha_k$: test filter weights
- $\beta$: enhancement factor blending function
- $\Gamma$: turbulence model blending function
- $\Delta$: mesh scale
- $\delta_{ij}$: Kronecker delta
$\varepsilon$  turbulent dissipation
$\kappa$  Von Karman constant
$\mu$  dynamic viscosity
$\nu$  kinematic viscosity
$\dot{\omega}_s$  species production rate
$\rho$  density
$\tau_{ij}$  stress tensor

**Superscripts**

- c  convective component
- p  pressure component
- R  resolved
- S  sub-grid
- n  time level
- k  sub-iteration level

**Subscripts**

- i,j,k  cell indices, spatial coordinates
- t  turbulent
- max  maximum
- min  minimum
- mix  mixture
- SGS  sub-grid scale
- s  species
- st  stoichiometric
- 1/2  cell interface
- L,R  left and right states
- $\infty$  free-stream conditions
Accents

\vec{v} \quad \text{vector}
\hat{v} \quad \text{test-filtered quantity}
\bar{v} \quad \text{time-averaged quantity}
\tilde{v} \quad \text{density-averaged quantity}
\prime \quad \text{time-fluctuation}
\" \quad \text{mass-fluctuation}

Abbreviations

ANN \quad \text{artificial neural network}
BSL \quad \text{baseline}
CV \quad \text{control volume}
DES \quad \text{detached eddy simulation}
ENO \quad \text{essentially non-oscillatory}
ILU \quad \text{incomplete lower/upper}
LES \quad \text{large eddy simulation}
LDFSS \quad \text{low-diffusion flux-splitting scheme}
LSM \quad \text{least-squares minimization}
LSM-FS \quad \text{LSM- filtered sources}
LSM-FS-H \quad \text{LSM- filtered sources with heat}
LSM-SS \quad \text{LSM- scale-similarity}
LSM-SS-H \quad \text{LSM- scale-similarity with heat}
MMD \quad \text{minmod}
NS \quad \text{number of species}
OSP \quad \text{‘optimal single point’}
PPM \quad \text{piecewise parabolic method}
RANS \quad \text{Reynolds-averaged Navier Stokes}
TKE \quad \text{turbulent kinetic energy}
TVD \quad \text{total variation diminishing}
Chapter 1

Introduction

In this chapter, we will define hypersonics and the problems and challenges faced in developing the propulsion systems for hypersonic vehicles. The motivation of designing such vehicles will be discussed as well as the role CFD has played throughout history in supporting such developments. This will lead to a discussion on the modern techniques used in high speed reactive simulations and some of the challenges being faced today. These challenges provide the motivation of this work, one being the development of closure models for turbulent combustion.

1.1 Hypersonic Propulsion

Hypersonic is generally defined by flight conditions greater than Mach 5. It is at this point that aerodynamic heating begins to play a major role in the physics of the flow. Historically, hypersonics has been relevant since the 1940s as the German wartime V-2 rocket flew at speeds greater than Mach 5. Since then, the hypersonic flight regime has played a role in several applications. Perhaps the most common application is in the use of aerodynamic braking in re-entry vehicles. These un-powered orbital vehicles return to Earth at extreme speeds (often much greater than Mach 5) at which point chemical dissociation occurs due to extreme heating. In order to endure these extremely hostile conditions, specially designed heat shields were designed to ensure the craft didn’t burn up during re-entry.

In the case of powered flight, hypersonic flight conditions are experienced by launch vehicles and ballistic missiles. Traditionally, these types of vehicles are powered by rockets; however, alternative air breathing propulsion systems have been and still are being pursued. In the case of rocket powered vehicles, the oxidizer is carried aboard the vehicle, while the latter case obtains oxidizer from the surrounding atmosphere. The obvious advantage of air breathing propulsion lies in the fact that no oxidizer needs to be carried. This means that a well designed air breathing propulsion system would have a higher
specific impulse than the rocket powered counterpart as well as a longer range. An air breathing propulsion system also has the advantage of dynamic thrust control whereas any rocket thrust variation must be designed and planned ahead of time. The main drawback in these high speed air breathing propulsion systems is getting to the correct speeds required for them to operate properly.

There are essentially two high speed air breathing propulsion designs: turbojet engines and ramjet/scramjets. Turbojet engines are designed to operate at subsonic speeds and are comprised of a compressor, a combustor, a turbine and a nozzle. The compressor is used to compress the incoming air to high enough pressures for optimal combustion to occur in the combustion chamber. The hot products pass through a turbine to extract some energy to power the compressor before being further expanded through the nozzle to provide thrust for the aircraft. Depending on the design, these engines can operate over a wide range of speeds allowing for a single stage engine from takeoff to supersonic speeds; although the engine performs poorly at low speeds. At flight speeds around Mach 3, the compressor is no longer needed as compression due to shock waves is sufficient enough to ensure optimal combustion. This leads to the design of ramjet/scramjet engines. The ramjet engine operates at supersonic speeds at which a series of oblique and eventually normal shock waves result in compression of the oxidizer to pressures required for combustion. The shocks also result in a subsonic flow within the combustor. Since there is no compressor, the turbine is also not needed, thus this system requires no moving parts. The hot combustion products are then simply expanded out of a nozzle to provide greater thrust compared to a turbojet engine. Clearly, there is an underlying problem to this system; it relies on the high speeds of the incoming airstream to generate a shock-system to compress the air.

Due to this reliance on high freestream air speeds, a ramjet engine cannot operate efficiently at Mach numbers lower than M=2. There is also an upper limit to the operating speeds. Depending on the design of the inlet, there is some Mach number at which the engine will begin to lose efficiency due to total pressure losses, or begin to encounter high amounts of stresses due to very strong shocks. This occurs around Mach 5. To avoid this, an alternative is a supersonic combusting ramjet engine (or scramjet). These engines utilize a series of oblique shocks to allow for some initial compression and deceleration. However, the flow still remains supersonic, so the fuel-air mixing and combustion must occur at much shorter residence times. Controlling this complex combustion process is a major challenge for the design of scramjet engines.

1.2 Brief history of CFD in Hypersonics

This section summarizes the developments of computational fluid dynamics in Hypersonics since the 1960s. A more thorough summary of the history of CFD in hypersonics can be found in [1, 2]. In 1965, NASA Langley research center initiated the Hypersonic Research Engine (HRE) project to develop high speed air breathing technology for the propulsion systems of hypersonic cruise vehicles. The goal of the
project was to flight test a hydrogen fueled pylon mounted scramjet engine on the X-15 research plane. Although the project never reached flight demonstration because the X-15 was eventually canceled, ground based testing continued. The Navy also sponsored a scramjet propulsion program at the Applied Physics Lab of Johns Hopkins University (JHU/APL). This work increased in the 1960s and was directed towards development of a shipboard missile system using a scramjet combustor. This project continued until 1977. Both projects, along with interest in the problem of re-entry vehicles from space, provided the early motivation for the development of computational techniques for the modeling of supersonic reacting flows. Later, in the 1980s, the NASP program provided further motivation and funding leading to more developments. This eventually lead to fully implicit, 3D codes capable of handling finite rate chemical kinetics and vibrational non-equilibrium. Shortly after the end of the NASP program, the Hyper-X program was initiated which saw the develop of some of the modern codes and techniques used today.

Computational techniques were fist applied to study supersonic reacting flow fields in a scramjet combustor in the 1970s. The works of Ferrie, Moretti, Edelman and Dash were some of the first to solve supersonic flow paths [3–7]. Other programs were simultaneously being developed to solve external high speed flow problems such as the work by MacCormack [8]. These codes were eventually adapted to internal reacting flows as well. The same period saw work by Briley and McDonald [9] as well as Beam and Warming [10] to develop implicit techniques for Navier-Stokes solvers. These implicit methods were used to model the inlet flow fields while explicit methods were applied to the study of the combustor flow. Early on it was common practice to use equilibrium chemistry to model the fuel-air reactivity. Using this assumption, one of the first scramjet flow fields using a 2D model engine was carried out by Drummond [11] with the TWODLE combustor program.

NASA and JHU/APL hypersonic programs continued into the 1970s, and involved both computational and ground based testing. In 1985, there was a joint effort between the Air Force and NASA to start development of a single stage to orbit launch vehicle using hypersonic air breathing technology called the National AeroSpace Plane (NASP). The program began in 1982 as a highly classified Defense Advanced Research Project Agency project called Copper Canyon. One of the first effort in this program was extension of the TWODLE code [12], which evolved into the SPARK combustion program. This program would be used in early studies of the NASP flow path. A major extension in capability of the program was performed by Carpenter in the addition of finite-rate chemistry and extension to three dimensions [13]. In addition to NASA sponsored codes, other codes developed by Spalding, Dash and MacCormack remained popular. Spalding’s SHIP code would be used to design studies of different scramjet configurations [14], while Dash’s SCORCH code was used for in depth studies of experiments used to design the NASP propulsion system [15].

The NASP era also saw further motivation in the need to model external flows for NASP as well as re-entry vehicles. Methods were developed to model strongly shocked flows with reacting air chemistry.
MacCormack and Candler would develop flux split algorithms for modeling high speed flows that were ionized and in thermodynamic and chemical non-equilibrium [16, 17]. Success in modeling the reacting air flows made it clear that the code could easily be modified to simulate combustion chemistry of an internal scramjet combustor flow field as well. Meanwhile a code was also developed by Grossman, Walter, and Cinnella to model high speed reacting flows. The initial code solved the Euler equations for non-reacting flow, but included real gas effects [18]. After success in applying the code to a 1-D shock tube problem, the code was extended to a 2-D solver that used an implicit method. They would further add capabilities to handle vibrational and chemical non-equilibrium by adding species and vibrational energy conservation equations to the system [19].

By the early 1990s, the NASP program was winding down. Fortunately, it was followed shortly by the Hyper-X program a few years later. In 1995, the Hyper-X program began as a joint effort between NASA Langley and the Dryden Research Center. The program had the specific goal of flight testing a scramjet powered vehicle. The flight plan involved using a B-52 aircraft to carry the Hyper-X vehicle along with a Pegasus rocket to operating altitudes. Upon reaching the desired altitude, the Hyper-X vehicle is released and accelerated to hypersonic speeds by the rocket. One the rocket fuel is expelled, it is released and the scramjet engine is used to power the vehicle. Similar to the NASP program, experiments were costly and limited to ground testing. Therefore, computational methods were key to design of engine flow paths as well as to gaining an in-depth understanding of the critical regions of the flow. The developments in this period would lead to many of the programs used today for both fundamental and design studies.

One of the first efforts to develop a code for a hypersonic scramjet simulation began in 1987 with the GASP code. The GASP program was capable of solving steady and unsteady Euler equations as well as the Navier-Stokes equations. The code included several options including preconditioning, approximate factorization, line Gauss Siedel, GMRES, mesh sequencing and multi-grid capabilities. The code also allowed for different flux-splitting methods including Roe [20] and van Leer [21] flux splitting as well as central differencing with artificial viscosity. In addition, turbulent flows could be modeled using algebraic or two-equation turbulence models with wall function options. GASP was also equipped with a database of 455 reactions and 34 species for handling air, hydrogen-air, and hydrocarbon chemical kinetics. The GASP code was validated for several internal and external flows [22–24].

Another effort to develop a code for these applications began in 1992 at NASA Langley Research Center with the LARCK program (Langley Algorithm for Research in Chemical Kinetics). The LARCK program would serve as the predecessor for the Viscous Upwind aLgorithm for Complex flow ANalysis or VULCAN. The original LARCK code had capabilities that included solving the Reynolds averaged Navier-Stokes (RANS) equations with several options for turbulence modeling as well as Arrhenius based chemical reaction models. VULCAN built on these capabilities by including options for Roe flux splitting or Edwards’ low diffusion flux splitting scheme [25]. Further, VULCAN would include...
time-derivative preconditioning to handle low speed flows [26] as well as additional turbulence models that were being developed alongside VULCAN. One of the early uses of the VULCAN code was the investigation of advanced fuel injection methods for scramjet engines [27]. Work has continued on the VULCAN code over the past decade, focusing on the addition and assessment of LES and hybrid LES/RANS capabilities [28]. VULCAN has been used in LES/RANS analysis of several experimental and fundamental studies, including those documented in [29, 30].

1.3 Modern Techniques: RANS, LES and DNS

Today, one of the largest challenges in the supersonic combustion CFD community is the treatment of turbulence and its effect on the mixing and combustion processes. In this section, we discuss the difference of four different models for solving turbulent reacting flow problems. The first are RANS techniques, which are considered the state of the practice. This first generation model has been incorporated into many CFD codes worldwide, such as the NASA VULCAN solver, Aerosoft’s GASP program, NCSU’s REACTMB platform, and Metacomp Technologies’ CFD++ software. The community is moving to development of second-generation hybrid LES/RANS and third-generation LES techniques to address some of the shortcomings of RANS solvers. The fourth is DNS or direct numerical simulation of the Navier-Stokes equations which yields the best results, but is impractical due to the extremely high computational cost.

The first generation model, considered state of the practice today, solves the Reynolds averaged Navier-Stokes equations. These equations are derived by filtering the Navier-Stokes equations over time. The flow variables are decomposed into mean and fluctuation parts. These equations require closure for the Reynolds stresses which are the terms that remain due to filtering of combinations of the fluctuating components of the velocities. Many of the models developed to provide closure to these terms require many assumptions or calibration for different flow problems. The primary advantage of RANS techniques is that the simulations are relatively cheap as there are no mesh refinement requirements needed to resolve a certain level of turbulent motion. However, there are many drawbacks. First, since the models require several assumptions and calibration of model constants, there is no reason to expect a flow solver to work well for different types of flow or different flow conditions. Also, since the RANS equations are time averaged, it is difficult to apply these techniques to study highly transient processes such as supersonic combustion or mode transition in a dual mode combustor.

Large-Eddy Simulation (LES) addresses many of the concerns of RANS techniques. In LES, the Navier-Stokes equations are spatially filtered to solve for the filtered component of the velocity field with the effects of the residual component being modeled. The spatial filter is often implicitly chosen to be equal to the mesh scale. Since individual cells are used to capture the eddy structures being resolved, the size of the structures being captured are actually no smaller than $2\Delta$, and it is often possible that
the effective filter width is significantly greater than the mesh spacing. Therefore, this requires mesh refinement to the largest scale of motion that needs to be resolved. The primary advantage of LES over RANS is that this spatially filtered field is both three dimensional and time-dependent, and this field represents the motion of the largest eddies. Also, since the larger eddies are the ones that are geometry and case dependent, the effect of the non-isotropic turbulence is being captured. The effect of the smaller (called subgrid scales or SGS) is assumed to be more universal and should be easier to model. The primary drawback in LES comes from the mesh requirements to resolve the largest eddy structures. This is especially true in regions near the walls where the largest scales of turbulence decrease with decreasing wall distance in all directions. Further, the range of turbulent spatial scales that needs to be resolved widens with increasing Reynolds number, as the flow must break down into finer structures to allow for viscous forces to compensate for the increased inertial forces.

Due to the expensive mesh requirements, the use of pure LES is limited today, as the computational cost makes it impractical. One method to reduce the cost of using LES methods is to cut the cost of the mesh wall-refinement. This can be achieved by using RANS methods in near-wall regions and LES in all other regions. The required mesh resolution near the walls will be significantly reduced by using RANS type corrections to the momentum equations. This method is referred to as Hybrid LES/RANS. The primary issue with Hybrid LES/RANS techniques is in the blending of the two schemes, and where this switching point should occur. Hybrid LES/RANS methods are still in the stages of development and validation but have been implemented into some codes including the VULCAN solver and NCSU’s REACTMB.

The final solution method that accounts for turbulent effects is direct numerical simulation (DNS) of the Navier-Stokes equations. DNS requires that the mesh resolve all scales of turbulent motion. Since DNS resolves all the turbulent scales, no closure models are required and the flow is solved for the time accurate field of variables. The computational cost of DNS is even greater than LES and can be approximated by the cube of the Reynolds number of a flow. This makes it feasible for only low or moderate Reynolds number with today’s computer technology. Today, DNS techniques are usually reserved for academic studies used to assess LES models. Further discussion on RANS/LES including the models and equations are discussed in Section 2.4

1.4 NCSU’s REACTMB Code

The solver used in this work is NCSU’s REACTMB solver; the code is a compressible, reactive, viscous flow solver that uses finite volume methods to solve flows on structured multi-block grids. REACTMB’s development began with a RANS code developed by Dr. Jack Edwards in the mid-1990’s [31]. The original code was extended to a 3D version and used in vector computers [32]. Simultaneously, another version was developed to solve 3D flows on multi-block structured meshes in parallel. Some work using
this version of REACTMB is reported in [33–35].

Later, with an increase in available computing power, hybrid LES/RANS methods were revisited. Developments were carried out by Drs. X. Xiao and J. Edwards at NC State to implement methods for carrying out 3D hybrid LES/RANS simulations with more general multi-blocking and MPI parallelism. Previous work in simulating high-speed, turbulent, reactive flows using this version of REACTMB can be found in [2, 36–40]. In addition to the original purpose of simulating high-speed reacting flows, a number of variations of REACTMB exist that can handle low-speed flows, multi-phase flows, electro-sprays, re-entry flows, and flows in thermal non-equilibrium. Some results of these variants are presented in [41–46]. The governing equations and numerical methods used in the REACTMB code will be discussed in chapters 2 and 3.

1.5 Motivation for this Work

The Hypersonic CFD lab at NC State has a general goal of developing a new generation of hybrid LES/RANS methods that improve on the state of the practice and are economical to implement. Some of the issues addressed by the group includes the need to develop advanced subgrid scale and RANS-type turbulence closures as well as modern chemistry models and efficient computational techniques. Among these areas, this work is aimed at developing subgrid scale models designed to account for the effects of turbulence on chemical reactivity [47].

The primary application considered in this work is scramjet combustion; these high speed reactive flows are characterized by the coupling of several different complex physical phenomenon. This includes reaction chemistry when combustion occurs as well as significant compressibility effects (such as shock / plume interactions) due to very high Mach numbers. Further, the flows are characterized by high turbulence levels as well as convective time scales that are comparable to chemical time scales. These effects, in addition to highly transient events such as ignition, extinction, blow-off and moving shock trains, imply that time-accurate LES with finite-rate chemistry is the most appropriate method for studying these flows. Finite-rate chemistry is favored for these applications opposed to the other methods such as tabulated chemistry approaches; the latter trade the cost of evolving a large number of species for a reduced set of conserved scalars (such as mixture fraction) and/or progress variables. Although many variants exist, usually tabulated chemistry methods involve presumed flame structures that satisfy some prescribed distribution. Clearly, the limitation of such models is that they can only be applied to specific problems; this work is concerned with developing methods that can capture a complete picture of the physics behind general reactive flow problems with little to no modification for different combustion regimes.

The state of the practice when using finite-rate chemistry in LES is to assume “laminar chemistry”
due to its simplicity. This involves modeling the filtered chemical production rates as equal to the production rates evaluated based on resolved quantities \( \dot{\omega}_s(q) = \dot{\omega}_s(\bar{q}) \). While acceptable results can be obtained using this assumption [36, 38, 39], the general trend is that laminar chemistry (LC) overestimates reactivity. This leads to flame temperatures that are higher than typically measured using non-intrusive diagnostics. Despite this, it is not certain that the effect of turbulent fluctuations is to always decrease reactivity. The fact that chemistry occurs at the smallest scales implies that the smallest turbulent scales that are not being resolved must have some effect on the chemical source terms. This means that the closure model for chemical production rates should take into account some correction for the action of the turbulent fluctuations occurring at the subgrid-scale.

Several advanced subgrid models for combustion are available. These include filtered density function models, one-dimensional turbulence (ODT) models, direct quadrature methods, etc. A review of these models are given in Chapter 4. The problem with most of these closure models, is that they can be expensive and are often difficult to implement. Filtered density function methods, for example, require evolution of several realizations of the flow which are then ensemble averaged or tracking of a large number of stochastic particles to provide a subgrid scale average to close the LES equations. ODT methods require refinement in directions that maximize scalar gradients to capture the influence of subgrid-scale effects on chemistry and diffusion. Both of these models involve significant additional cost to the already expensive cost of LES. The goal of this work is to develop closure models that add negligible expense to the computation, but provide a consistent, quantifiable improvement in predictive capability relative to ‘laminar chemistry.’ The form is as follows, where the enhancement factor, \( f \), is designed to account for the effect of the unresolved fluctuations on the apparent reactivity for a given mesh scale.

\[
\overline{\dot{\omega}_s(q)} = f(q, \Delta, \ldots) \dot{\omega}_s(\bar{q})
\]

Previous work by our group [2, 40, 48] has focused on this issue. However, those studies involve models in which a traditional \textit{a priori} analysis was used in development. The traditional \textit{a priori} approach involves comparing chemical production rates from a fine-mesh simulation with production rates evaluated from the filtered field of fine-mesh data. Part of this study is to develop a modified \textit{a priori} analysis in which a sequence of grids is used to study the effects of grid resolution on chemical production rate prediction. By studying the change in chemical production rates for different grid resolutions, the effect of the subgrid portion can be quantified and modeled. Taking the finest grid resolution as the ‘truth model’, the filtered chemical source terms from the fine grid level to the coarse grid can serve as a model for the filtered production rates. This leads to the use of least-squares minimization between the filtered fine grid chemical production rates and the production rates determined using laminar chemistry as the basis for the new family of closure models derived in this work. The modified \textit{a priori} approach is discussed in Section 4.9.2; the new models are defined in Section 4.10. Results comparing the effects of the different closure models are discussed throughout Chapter 5.
Chapter 2

Governing Equations

In this chapter, the governing equations for turbulent reactive flows are defined. The derivation begins with the basic equations of conservation governing all fluid flows followed by a multi-species extension and ending with chemical and turbulence closures.

2.1 Basic Conservation Equations

The basic equation that governs any fluid property can be expressed in tensor notation as shown in Eq. 2.1. From a finite volume perspective, this represents the balance of the temporal evolution within the volume with the advection of the fluid property through the control surface and the sources acting on the volume.

\[
\frac{\partial q}{\partial t} + \frac{\partial}{\partial x_j} (q u_j) = S
\]  

(2.1)

In Eq. 2.1, \( q \) represents any conserved flow property, such as mass, momentum or energy, per unit volume. The first term is the unsteady term which accounts for the temporal change of \( q \) at each point in the flow field. The second term is the flux derivative which accounts for the change in \( q \) due to accumulation or depletion of \( q \) due to fluid being ‘carried in’ or ‘carried out’ of the control volume. The term on the right hand side is the source term which accounts for changes in \( q \) due to external sources. The sources will vary depending on the conserved property.

In describing the motion of a fluid, three properties are required to fully describe the flow field. These are mass, momentum, and energy. Applying Eq. 2.1 to these properties results in the equations expressing the conservation of density (\( \rho \)), momentum per unit volume (\( \rho u_i \)), and the total energy per
unit volume $[\rho(e + \frac{u_i u_i}{2})]$ as described below.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{2.2}
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2.3}
\]

\[
\frac{\partial}{\partial t} \left[ \rho \left( e + \frac{u_i u_i}{2} \right) \right] + \frac{\partial}{\partial x_j} \left[ \rho u_j \left( e + \frac{u_i u_i}{2} \right) \right] = -\frac{\partial q_j}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} \tag{2.4}
\]

Eqs. 2.2 - 2.4 are the compressible Navier-Stokes conservation equations which govern fluid flow. This formulation neglects body forces (such as gravity) and radiative energy transfer effects as these are negligible for the conditions of this work. It is noted that Eq. 2.3 is actually a vector of three scalar equation for each Cartesian coordinate direction, while the continuity and energy equations are scalar equations. The continuity equation has no sources while pressure and viscous forces are included as the source terms to the momentum equation. There are three source terms in the energy equation representing the effects of heat conduction, pressure work, and viscous work. The pressure work term can be moved to the left-hand side to be included in the spatial flux term, resulting in the flux variable containing enthalpy rather than total energy.

\[
\frac{\partial}{\partial t} \left[ \rho \left( e + \frac{u_i u_i}{2} \right) \right] + \frac{\partial}{\partial x_j} \left[ \rho u_j \left( e + \frac{u_i u_i}{2} \right) \right] = -\frac{\partial q_j}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} \tag{2.5}
\]

It is clear that equations of state are needed to define the enthalpy $h$, the viscous stress tensor $\tau_{ij}$, heat transfer $q_j$, and pressure $p$ in order to fully close this system of equations. Further we must extend the system of equations to consider multi-species mixtures of gases since the work considered involves reactive chemistry. This will be discussed in the following section.

### 2.2 Extension for Multiple Species

The standard Navier-Stokes equations are used to govern the flow of a single fluid with a single equation for viscosity, enthalpy, etc. The simulations considered here involve the mixing and combustion of several different species, each with its own properties. The properties of the mixture are a combination of the properties of the individual species that compose the mixture. An extension to the above equations is required to include these effects. The new system will require tracking of the individual components of the mixture and the changes in their composition due to mixing as well as chemical reactivity.

To keep track of the composition of each of the individual species, the species continuity equation is used as given in Eq. 2.6. Here, $s$ ranges from 1 to NS, adding one equation for each individual species considered in the simulation. The first term is the temporal change of the species density, while the
second term accounts for the advection and diffusion of the species. The source term on the right-hand side is the species production rate due to chemical reactions.

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho_s (u_j + V_{s,j}) \right] = \dot{\omega}_s$$  \hspace{1cm} (2.6)

The summation of all of the species conservation equations will result in Eq. 2.2 and so the total mass of the system is still conserved. This property requires that \(\sum_{s=1}^{NS} \dot{\omega}_s = 0\).

The mixture momentum equation is given by Eq. 2.7.

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho_i u_i + \sum_{s=1}^{NS} \rho_s V_{s,i} V_{s,j} \right] = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$  \hspace{1cm} (2.7)

The primary difference here is that the momentum flux due to the diffusion of the mixture species is included. In most cases, this term is neglected since normally \(V_{s,i} \ll u_i\). Therefore, the mixture momentum reduces to Eq. 2.3.

The mixture energy equation must keep track of the total energy of the mixture, accounting for the effects of energy transport from advection, diffusion, conduction and surface forces. Assuming the mixture consists of thermally perfect, ideal gases that are in thermal equilibrium, the mixture energy equation can be defined as shown in Eq. 2.8.

$$\frac{\partial}{\partial t} \left[ \sum_{s=1}^{NS} \rho_s e_s + \frac{1}{2} \rho u_i u_i \right] + \frac{\partial}{\partial x_j} \left[ u_j \left( \sum_{s=1}^{NS} \rho_s h_s + \frac{1}{2} \rho u_i u_i \right) \right] =$$

$$-\frac{\partial q_j}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \sum_{s=1}^{NS} \rho_s h_s V_{s,j} \right)$$  \hspace{1cm} (2.8)

Again, it is clear that Eqns. 2.6, 2.7, and 2.8 require additional equations to provide closure. These are defined below.

The mixture density is simply the summation of the individual species densities.

$$\rho = \sum_{s=1}^{NS} \rho_s$$  \hspace{1cm} (2.9)

The species diffusion velocity is defined based on Fick’s Law as shown in Eq. 2.10, where Sc is the Schmidt number (usually set to 0.5) and \(Y_s\) is the species mass fraction.

$$\rho_s V_{s,j} = -\frac{\mu}{Sc} \frac{\partial Y_s}{\partial x_j}$$  \hspace{1cm} (2.10)
The species mass fraction is defined as the ratio of species density to mixture density.

\[ Y_s = \frac{\rho_s}{\rho} \quad (2.11) \]

Based on Dalton’s Law, the pressure of the mixture is defined as the sum of the partial pressures.

\[ p = \sum_{s=1}^{NS} p_s \quad (2.12) \]

The partial pressure for each species is determined using the ideal gas law. \( R_s \) is the species gas constant which is the universal gas constant divided by the species molecular weight.

\[ p_s = \rho_s R_s T \quad (2.13) \]

\[ R_s = \frac{R_u}{M_{0,s}} \quad (2.14) \]

The internal energy per unit mass of each species is given by Eq. 2.15, where the species enthalpy is given by Eq. 2.16. Note that \( h_{f,s}^0 \) is the standard enthalpy of formation for species \( s \) at the reference temperature \( T_{ref} \).

\[ e_s = h_s - \frac{p_s}{\rho_s} \quad (2.15) \]

\[ h_s = h_{f,s}^0 + \int_{T_{ref}}^{T} c_{p,s}dT \quad (2.16) \]

The integral in Eq. 2.16 requires a defined relationship between the species specific heat capacities and temperatures. In this work, the relationship is determined based on the McBride curve fits [49]. The curve-fit database contain coefficients \( A_{i,s} - E_{i,s} \) that are used as shown in Eq. 2.17 to determine species specific heat capacities for a given temperature.

\[ c_{p,s} = R_s \left[ A_{i,s} + B_{i,s}T + C_{i,s}T^2 + D_{i,s}T^3 + E_{i,s}T^4 \right] \quad (2.17) \]

The curve-fit consists of two branches, meaning that there are two sets of coefficients for each species with one branch being valid at a lower temperature range and the other being valid at higher temperatures. The standard heats of formation are also accounted for by the McBride database. Thus, \( c_{p,s} \) and therefore \( h_s \) can be determined based on the fits within the valid temperature range. The mixture enthalpy and energy can be formulated as shown below.

\[ h = \sum_{s=1}^{NS} Y_s h_s \quad (2.18) \]
\[ e = \sum_{s=1}^{NS} Y_s e_s \] (2.19)

The mixture molecular viscosity is determined based on Wilke’s [50] semi-empirical relationship given in Eq. 2.20, where \( \phi_{ij} \) is defined by Eq. 2.21.

\[ \mu = \mu_{mix} = \sum_{i=1}^{NS} \frac{X_i \mu_i}{\sum_{j=1}^{NS} X_j \phi_{ij}} \] (2.20)

\[ \phi_{ij} = \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_{w,i}}{M_{w,j}} \right)^{1/4} \right]^2 \]

\[ \sqrt{8 \left( 1 + \frac{M_{w,i}}{M_{w,j}} \right)} \] (2.21)

The equation above requires mole fractions which are defined by Eq. 2.22.

\[ X_i = \frac{Y_i}{M_{w,s}} \sum_{s=1}^{NS} \frac{1}{Y_i / M_{w,i}} \] (2.22)

The heat transfer vector is formulated by Fourier’s law of heat conduction, extended for multiple species as shown in Eq. 2.23, where the Prandtl number \( Pr \) is normally set to 0.72.

\[ q_j = q_{j,mix} = -\frac{\mu}{Pr} \left( \sum_{s=1}^{NS} Y_s c_{p,s} \right) \frac{\partial T}{\partial x_j} \] (2.23)

Finally, the viscous stress tensor needs to be defined. The tensor is evaluated by assuming a Newtonian fluid and invoking Stokes’ hypothesis to yield Eq. 2.24.

\[ \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \] (2.24)

To summarize, the final form of the Navier-Stokes equations for a compressible mixture of thermally-perfect, reactive gases is given below. Eqns. 2.25 through 2.27 consist of \((NS+4)\) equations in 3D space. However, still required are methods for handling reactivity and turbulence which will be given in the following sections.

\[ \frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho_s (u_j + V_{s,j}) \right] = \omega_s \] (2.25)

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \] (2.26)
\[
\frac{\partial}{\partial t} \left[ \sum_{s=1}^{NS} \rho_s e_s + \frac{1}{2} \rho u u_i \right] + \frac{\partial}{\partial x_j} \left[ u_j \left( \sum_{s=1}^{NS} \rho_s h_s + \frac{1}{2} \rho u u_i \right) \right] = \\
- \frac{\partial q_j}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \sum_{s=1}^{NS} \rho_s h_s V_{s,j} \right)
\]

(2.27)

### 2.3 Chemical Reactivity

Chemistry in REACTMB is handled based on the law of mass action, which relates the production and depletion of individual species to the known composition of the mixture. The general form of any chemical reaction is given by Eq. 2.28 where \( N_s \) is the chemical name for a species \( s \) and the stoichiometric coefficients for the reactants and products are \( \nu'_s \) and \( \nu''_s \), respectively. For this general reaction, the law of mass action can be expressed as shown in Eq. 2.29 where \( \dot{\omega}_s \) is the time rate of change of the species mass density and \( \hat{\rho}_s = \rho_s / M_{w,s} \) is the molar density of a particular species. The rate of reaction, \( RR_i \) is given by Eq. 2.30.

\[
\sum_{s=1}^{NS} \nu'_s N_s \Leftrightarrow \sum_{s=1}^{NS} \nu''_s N_s
\]

(2.28)

\[
\dot{\omega}_s = M_{w,s} \sum_{i=1}^{NR} (\nu'_s - \nu''_s)RR_i
\]

(2.29)

\[
RR_i = k_{f,i} \prod_{j=1}^{NS} (\hat{\rho}_j)^{\nu'_j} - k_{b,i} \prod_{j=1}^{NS} (\hat{\rho}_j)^{\nu''_j}
\]

(2.30)

It is also noted that the ‘positive’ and ‘negative’ source terms can be calculated separately. The ‘positive’ sources are defined as the summation of the reaction rates that contribute to the net production of a species while the ‘negative’ source terms are the composed of the reaction rates that contribute to the net consumption of a species. Note that the forward and backward rate coefficients \( k_f \) and \( k_b \) have units that depend on the order of the reaction.

\[
\dot{\omega}_s^+ = \sum_{i=1}^{NR} \left( \nu''_s k_{f,i} \prod_{j=1}^{NS} (\hat{\rho}_j)^{\nu'_j} + \nu'_s k_{b,i} \prod_{j=1}^{NS} (\hat{\rho}_j)^{\nu''_j} \right)
\]

(2.31)

\[
\dot{\omega}_s^- = -\sum_{i=1}^{NR} \left( \nu''_s k_{b,i} \prod_{j=1}^{NS} (\hat{\rho}_j)^{\nu'_j} + \nu'_s k_{f,i} \prod_{j=1}^{NS} (\hat{\rho}_j)^{\nu''_j} \right)
\]

(2.32)

\[
\dot{\omega}_s = \dot{\omega}_s^+ + \dot{\omega}_s^-
\]

(2.33)

The forward rate coefficients for reaction \( i \) are calculated based on the Arrhenius equation shown in Eq. 2.34. The Arrhenius constants \( A_i, \eta_i \), and the activation energy \( E_{a,i} \) are provided from reaction
mechanisms such as those provided by Burke et al. for hydrogen combustion [51].

\[ k_{f,i} = A_i(T)^{\eta_i} \exp \left[ \frac{-E_{a,i}}{R_u T} \right] \] (2.34)

Backward rate coefficients are determined based on the equilibrium rate constant \( k_{eq,i} \) as shown in Eq. 2.35. The equilibrium constant is determined for each reaction based on the change in Gibbs free energy \( \Delta G_i \) as shown in Eq. 2.36. The change in Gibbs free energy is determined based on the McBride curve fits as shown in Eqns. 2.37 through 2.39.

\[ k_{b,i} = \frac{k_{f,i}}{k_{eq,i}} \] (2.35)

\[ k_{eq,i} = \left( \frac{101325}{R_u T} \right)^{(m_i''-m_i')} \exp \left( \frac{\Delta G_i}{R_u T} \right) \] (2.36)

\[ \Delta G_i = \sum_{s=1}^{NS} (v_{s,i}'' - v_{s,i}') g_s \] (2.37)

\[ g_s = h_s - T s_s \] (2.38)

\[ s_s = R_u \left[ A_s \ln T + B_s T + C_s T^2/2 + D_s T^3/3 + E_s T^4/4 + G_s \right] \] (2.39)

Next we incorporate equations to handle third-body reactions. These reactions are characterized by a third body species involved that aids in the dissociation of a molecule or in the recombination of molecules. The generic form of the third body reaction is shown in Eq. 2.40. The third body reactant, which can be any of the considered species, is denoted by \( M \), and it participates as an non-reacting collision partner.

\[ AB + M \rightleftharpoons A + B + M \] (2.40)

Using the law of mass action, we can define the chemical production rate for a dissociation reaction as shown in Eq. 2.41.

\[ \dot{\omega}_s = M_{w,s}(v_{s}'' - v_{s}') \sum_{i=1}^{NS} (k_{f,i}\hat{p}_i)\hat{p}_{AB} - \sum_{i=1}^{NS} (k_{b,i}\hat{p}_i)\hat{p}_A\hat{p}_B \] (2.41)

The forward and backward rates for this reaction are now scaled by the species third body efficiency as shown below.

\[ k_{f,i} = k_f(TB)_i \] (2.42)

\[ k_{b,i} = k_b(TB)_i \] (2.43)

Substituting the expression for the rate coefficients into 2.41 yields the source term for a single reaction as shown in Eq. 2.44.

\[ \dot{\omega}_s = M_{w,s}(v_{s}'' - v_{s}') \left[ k_f\hat{p}_{AB} - k_b\hat{p}_A\hat{p}_B \right] \sum_{i=1}^{NS} (TB)_i\hat{p}_i \] (2.44)
Summing over all of the dissociation / recombination reactions (ND), yields the contribution to the chemical source term due to third body dissociation reactions as shown.

\[ \dot{\omega}_s = M_{w,j} \sum_{i=1}^{ND} \left[ (v'_{s,i} - v'_{s,j}) \left[ k_{f,i} \hat{\rho}_{AB} - k_{b,i} \hat{\rho}_A \hat{\rho}_B \right] \sum_{j=1}^{NS} T B_i^j \hat{\rho}_j \right] \] (2.45)

Normally, chemically reactions are assumed to be functions of temperature alone. However, this is not always the case; some reactions are strongly influenced by pressure. This pressure dependence can be accounted for by blending the rate coefficients at high and low pressures to calculate the overall rate coefficient at a specified intermediate pressure. The forward rate constant for a given low pressure and high pressure is denoted by \( k_{f,0} \) and \( k_{f,\infty} \), respectively. The forward rate constant for a pressure dependent reaction is defined by Eq. 2.46, where the reduced pressure, \( p_r \), and function \( F \) are defined as follows. Note that these equations are closed as a function of temperature and the constants \( k_{f,0} \), \( k_{f,\infty} \), \( a \), \( T^* \), \( T^{**} \), and \( T^{***} \). This blending procedure was developed by Troe et al [52].

\[ k_f = k_{f,\infty} \left( \frac{p_r}{1 + p_r} \right) F \] (2.46)

\[ p_r = \frac{k_{f,0}}{k_{f,\infty}} \hat{\rho}_{mix} \] (2.47)

\[ \ln(F) = \left[ 1 + \left( \frac{\ln(p_r) + c}{n - d(\ln(p_r) + c)} \right)^2 \right]^{-1} \ln(F_{cent}) \] (2.48)

\[ c = -0.4 - 0.67 \ln(F_{cent}) \] (2.49)

\[ n = 0.75 - 1.27 \ln(F_{cent}) \] (2.50)

\[ d = 0.14 \] (2.51)

\[ F_{cent} = (1 - a) \exp \left( \frac{-T}{T^{***}} \right) + a \exp \left( \frac{-1}{T^*} \right) + \exp \left( \frac{-T^{**}}{T} \right) \] (2.52)

The equations above, along with those in Section 2.2, achieve full closure for a compressible mixture of reactive species. Required are chemical reaction mechanisms to provide the model constants for the rate coefficients. In this study, the chemical mechanism of Burke et al. [51] is used for hydrogen-air combustion while ethylene combustion is modeled using the Taitech-Princeton 22-species mechanism [53]. A two-step propane-air mechanism is used for the final case presented [54]. More information on these reaction mechanisms can be found in Appendix A. The next section will describe the equations used to account for the effects of turbulence.
2.4 Turbulence Closure

Turbulence occurs when the inertial forces dominate the flow to the extent that the molecular viscous forces cannot balance them in order to maintain a smooth response in regions of velocity gradients such as walls or in shear or wake regions. The result is a breakdown of the flow into a series of eddies, which can vary in size, in order to compensate for the flow inertia. These eddies are local regions where the molecules may be traveling with a net ‘bulk’ velocity but on a much finer scale, the motion is much more chaotic. The largest eddies can be broken up into a cascade of smaller eddies which individually have their own characteristic sizes, speeds and energy. Energy from the larger eddies is transferred down into the successively smaller eddies until the Reynolds number is small enough that the inertial and viscous forces balance, and an essentially laminar flow exists. This rate at which energy is transferred is called the energy dissipation rate, \( \varepsilon \). The smallest eddies are the smallest sections of the flow in which ‘order’ exists and the flow varies smoothly. If the length scales of the smallest eddies are resolved by a computational grid, then the solution of the Navier-Stokes equations (Eqns. 2.25 - 2.27) are valid and correspond to Direct Numerical Simulation (DNS). However, for very high Reynolds numbers, these length scales are incredibly small and would require a mesh resolution that would be impractical in the turbulent regions of the flow. Because of this issue, different techniques must be used to ‘filter out’ and model the effects of the turbulent fluctuations of the unresolved eddies. The two primary methods of choice are Reynolds Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) methods. In this work, all simulations are carried out using Hybrid LES/RANS techniques, the methods for which will be discussed in the following sections.

2.4.1 Large-Eddy Simulation

In large-eddy simulations (LES), the turbulent fluctuations are filtered out using a spatial filter. This means that the larger eddies are explicitly being resolved (thus the name large-eddy simulation) and the effects of the unresolved fluctuations that are being filtered out are modeled. Typically, LES takes the filter size to be the mesh scale. This means that the largest eddies that can be resolved have characteristic lengths on the order of the mesh scale. Any eddies smaller than this size act at the ‘sub-grid’ level and require modeling. A major assumption in LES is that the larger eddies that are resolved are those that are geometry dependent and the smaller eddies that are not being resolved are small enough that their behavior is more universal.

The spatial average of a space dependent, instantaneous variable \( q(x) \) can be performed using Eq. 2.53 where \( D \) is the complete domain over which \( q \) is defined and \( G \) is the filter weighting function with the property given in Eq. 2.54.

\[
\bar{q}(x) = \int_D G(x,x')q(x')dx'
\]  

(2.53)
\[
\int_D G(x,x') = 1 \quad (2.54)
\]

The distribution of the function \( G \) determines the filter width in which \( q \) is averaged. In LES, the width is normally taken to be the mesh width \( \Delta x \). The properties of the filtering is dependent on the type of filter; although many methods exist, one common filter is the box filter defined as shown below.

\[
G(x,x') = \begin{cases} 
\frac{1}{\Delta x} & \text{if } |x - x'| \leq \Delta x/2 \\
0 & \text{else}
\end{cases} \quad (2.55)
\]

Note that this filter gives equal weight to all data within the filter window. In three dimensions, the filtering operation is described as shown by Eq. 2.56.

\[
\bar{q}(x_1,x_2,x_3) = \int \int \int_D \left[ \prod_{j=1}^{3} G_j(x_j,x'_j) \right] q(x'_1,x'_2,x'_3) dx'_1 dx'_2 dx'_3 \quad (2.56)
\]

Favre averaging is used to reduce the number of unclosed terms resulting from the filtering operations. The density weighted, filtered quantity is given by Eq. 2.57. The decomposition of the variable \( q \) is composed of the ‘resolved’ or filtered quantity \( \bar{q} \) and the fluctuating or ‘sub-grid’ component \( q'' \).

\[
\bar{q} = \bar{\rho}q/\bar{\rho} \quad (2.57)
\]

\[
q = \bar{q} + q'' \quad (2.58)
\]

Substituting the decomposed variables and applying the spatial filter to the set of Navier-Stokes equations results in the compressible, reactive LES equations as shown below.

\[
\frac{\partial \bar{\rho} s}{\partial t} = \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} \left[ \bar{u}_j + \bar{V}_{s,j} \right] = \bar{\omega}_s \quad (2.59)
\]

\[
\frac{\partial (\bar{\rho} \bar{u}_i)}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} \quad (2.60)
\]

\[
\frac{\partial}{\partial t} \left[ \sum_{s=1}^{NS} \bar{p}_s e_s + \frac{\bar{\rho} \bar{u}_i \bar{u}_i}{2} \right] + \frac{\partial}{\partial x_j} \left[ \bar{u}_j \left( \sum_{s=1}^{NS} \bar{p}_s \bar{h}_s + \frac{\bar{\rho} \bar{u}_i \bar{u}_i}{2} \right) \right] =
\]

\[
-\frac{\partial \bar{q}_j}{\partial x_j} + \frac{\partial (\bar{u}_i \bar{\tau}_{ij})}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \sum_{s=1}^{NS} \bar{p}_s \bar{h}_s \bar{V}_{s,j} \right] \quad (2.61)
\]

Several terms require closure, including the filtered species diffusion velocity \( \bar{V}_{s,j} \), the filtered stress tensor \( \bar{\tau}_{ij} \), and the filtered heat flux \( \bar{q}_j \). These terms are split into the resolved and subgrid-scale
components as shown.

\[ \tilde{V}_{s,j} = V_{s,j}^R + V_{s,j}^S \]
\[ \tilde{\tau}_{ij} = \tau_{ij}^R + \tau_{ij}^S \]
\[ \bar{q}_j = q_j^R + q_j^S \] (2.62)

The resolved components are determined in the same fashion as the standard Navier-Stokes equations using the filtered (or resolved) variables.

\[ \bar{p}_s V_{s,j}^R = -\frac{\mu}{S_c} \frac{\partial \tilde{Y}_s}{\partial x_j} \]
\[ \tau_{ij}^R = \mu \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \] (2.63)

\[ \bar{q}_j = -\frac{\mu}{P_r} \left( \sum_{s=1}^{NS} \tilde{Y}_s \tilde{c}_{p,s} \right) \frac{\partial \tilde{T}}{\partial x_j} \]

The subgrid components are defined next, determined based on gradient diffusion and Boussinesq-type assumptions.

\[ \bar{p}_s V_{s,j}^S = -\frac{\mu_t}{S_c} \frac{\partial \tilde{Y}_s}{\partial x_j} \]
\[ \tau_{ij}^S = \mu_t \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu_t \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \] (2.64)

\[ \bar{q}_j = -\frac{\mu_t}{P_{rt}} \left( \sum_{s=1}^{NS} \tilde{Y}_s \tilde{c}_{p,s} \right) \frac{\partial \tilde{T}}{\partial x_j} \]

2.4.2 SGS Turbulence Modeling

The final closure required is for the subgrid-scale turbulent eddy viscosity, \( \mu_t \). The turbulent eddy viscosity must be modeled to account for the additional dissipation of the SGS fluctuations that are not being resolved. This is different from RANS, where the eddy viscosity is designed to account for all scales. Generally, this means that the eddy viscosity will be much smaller in LES compared to RANS.

The method used in REACTMB to calculate SGS eddy viscosity was developed by Lenormand [55] as an improvement to the Smagorinsky model [56]. The following equations summarize this method for determining \( \mu_t \), along with the necessary constants and relations.

\[ \mu_t = \bar{p}_s C_M \sqrt{\bar{\Omega}_D} c_{1/4} \Delta^{3/2} \] (2.65)
\[ \Delta = \sqrt{\Delta_x \Delta_y \Delta_z} \]
\[ q_c = \frac{1}{2} (\bar{u}_i - \bar{u})^2 \]  
(2.66)
\[ C_M = 0.06 \]

Note that \( \bar{u}_i \) is a test-filtered velocity. This test filter is defined for a generic variable as shown in Eq.
2.67. The quantity \( q_c \) uses a scale-similarity assumption to estimate the turbulent kinetic energy of the
subgrid-scales. This should result in the vanishing of the turbulent viscosity in the regions of the flow
where the turbulence is being fully resolved.
\[
\bar{q}_{i,j,k} = \frac{1}{2} q_{i,j,k} + \frac{1}{2} (q_{i+1,j,k} + q_{i-1,j,k} + q_{i,j+1,k} + q_{i,j-1,k} + q_{i,j,k+1} + q_{i,j,k-1})
\]  
(2.67)

### 2.4.3 LES-RANS Hybridization

As mentioned before, LES can be very expensive for high-speed, internal flows due to the necessity of
resolving the boundary layers. This cost can be reduced by utilizing hybrid LES/RANS methods. In or-
der to blend these techniques, a switching function is required. REACTMB uses a blending function (\( \Gamma \))
to switch between RANS and LES when an inner scale exceeds an estimate of an outer-layer turbulent
length scale. The blending function is defined so that \( \Gamma = 1 \) for RANS operation and \( \Gamma = 0 \) for LES.
The blending function is defined by Eq. 2.68. The constants required are defined as well.
\[
\Gamma = \frac{1}{2} \left[ 1 - \tanh \left( C_s \left( \frac{1}{2} \lambda_N - 1 \right) \right) \right] 
\]  
(2.68)
\[
\lambda_N = C_N \sqrt{10 + \frac{kR}{\nu \bar{\omega}}} \frac{\sqrt{\nu}}{c_\mu^{1/4} \kappa d \sqrt{\bar{\omega}}} 
\]  
(2.69)
\[ C_s = 15 \]
\[ C_\mu = 0.09 \]  
(2.70)
\[ C_N = 1.5 \]

In the above equations, \( \kappa \) is the Von Kármán constant (0.41), \( y_d \) is the wall distance, and \( k \) and \( \bar{\omega} \) are
ensemble averaged turbulent kinetic energy and specific dissipation rates, respectively. The resolved
turbulent kinetic energy, \( k_R \), can be determined as shown below.
\[
p k_R = \frac{1}{2} \left( \rho u_k u_k - \frac{\rho u_k \rho u_k}{\rho} \right) 
\]  
(2.71)
The ensemble averages are computed during the course of the simulation in the following manner, where \( n \) and \( n - 1 \) denotes the current and previous time steps. Here, \( t_{res} \) is the ‘residence’ time of a fluid particle in the domain \( (t_{res} = L/U_\infty) \) where \( L \) is the characteristic length of the domain and \( U_\infty \) is the inflow velocity. This formulation means that the blending function should vary in space and time due to non-equilibrium effects. Finally, the turbulent eddy-viscosity is defined as shown in Eq. 2.75 based on the blending function and the corresponding LES and RANS eddy viscosities.

\[
q^n = q^{n-1}(1 - A) + Aq^n
\]  
(2.72)

\[
A = \frac{\Delta t}{\tau}
\]  
(2.73)

\[
\tau = \begin{cases} 
\min(t, t_{res}) & t < 4t_{res} \\
t - 3t_{res} & t \geq 4t_{res} 
\end{cases}
\]  
(2.74)

\[
\mu_t = \left[ \Gamma \mu_{t,RANS} + (1 - \Gamma)\mu_{t,LES} \right]
\]  
(2.75)

### 2.4.4 RANS Turbulence Closure

Required for implementation of hybrid RANS/LES techniques is a method for calculating the RANS turbulent eddy viscosity, \( \mu_t \). The turbulent eddy viscosity for RANS requires the transport of turbulent kinetic energy as well. For determining these quantities, it is common to use a two-equation turbulence model. The variables used to describe turbulence within a flow are the turbulent kinetic energy, \( k \) and the energy dissipation rate, \( \varepsilon \), or the specific dissipation rate, \( \omega = \varepsilon/k \). A two equation model will involve adding two conservation equations in order to keep track of two of these variables. REACTMB has options for using the Menter BSL (baseline) model or the Menter SST model [57]. The Menter BSL model is a blend of the \( k - \omega \) and \( k - \varepsilon \) models. The blending is performed so that the \( k - \omega \) model is used in the viscous sublayer and the logarithmic regions of the boundary layer and the \( k - \varepsilon \) model is used in the wake region. This is done to take advantage of the superior performance of the individual models in these regions. The \( k - \varepsilon \) model is rewritten in terms of \( k \) and \( \omega \) in order to blend the models together.

For the Menter BSL model, the conservation equations for \( k \) and \( \omega \) are given below.

\[
\frac{\partial (\rho k)}{\partial t} + \bar{u}_j \frac{\partial (\rho k)}{\partial x_j} = \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \beta \bar{\rho} \omega k + \frac{\partial}{\partial j} \left[ (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right]
\]  
(2.76)
Table 2.1: Model Constants for Menter BSL Model

<table>
<thead>
<tr>
<th>Constant</th>
<th>k − ω (Model 1)</th>
<th>k − ε (Model 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>σ₀</td>
<td>0.5</td>
<td>1.0</td>
</tr>
<tr>
<td>σω</td>
<td>0.5</td>
<td>0.856</td>
</tr>
<tr>
<td>β</td>
<td>0.0750</td>
<td>0.0828</td>
</tr>
<tr>
<td>β*</td>
<td>0.09</td>
<td>0.09</td>
</tr>
<tr>
<td>γ</td>
<td>0.553</td>
<td>0.440</td>
</tr>
</tbody>
</table>

\[
\frac{\partial (\rho \omega)}{\partial t} + \bar{u}_j \frac{\partial (\rho \omega)}{\partial x_j} = \frac{\gamma}{v_t} \tau'_{i,j} \frac{\partial \bar{u}_i}{\partial x_j} - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_\omega) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \rho \sigma_\omega^2 \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \tag{2.77}
\]

Here, σ₀, σω, β, β*, and γ are model constants. Defining the set of constants as a vector φ₁ and φ₂ for the k − ω and k − ε models, respectively, the blending of the constants into a vector φ is performed for the Mentor BSL model as shown in Eq. 2.78.

\[
\phi = F_1 \phi_1 + (1 - F_1) \phi_2 \tag{2.78}
\]

The model constants are summarized in Table 2.1. The blending function, F₁, between the two model types is defined by Eqns. 2.79 - 2.81 while the eddy viscosity is defined as shown in Eq. 2.82. Note that y_d refers to the distance to the nearest wall.

\[
F_1 = \tanh(\text{arg}_1^4) \tag{2.79}
\]

\[
\text{arg}_1 = \min \left[ \max \left( \frac{\sqrt{k}}{0.09 \omega y_d}, \frac{500 \nu}{\omega y_d^2}, \frac{4 \rho \sigma_\omega^2 k}{C_{D_{k\omega}} y_d^2} \right) \right] \tag{2.80}
\]

\[
C_{D_{k\omega}} = \max \left[ 2 \rho \sigma_\omega^2 \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} + 10^{-20} \right] \tag{2.81}
\]

\[
\mu_\omega = \bar{\rho} k / \omega \tag{2.82}
\]

The second turbulence model available is the shear-stress-transport (SST) model that was also developed by Menter [57]. This model is nearly identical to the BSL model, but defines the eddy viscosity differently. The SST model defines the eddy viscosity based on turbulent kinetic energy and vorticity magnitude, as shown in Eq. 2.83, where Ω is the magnitude of the vorticity. According to [2], the SST model allows for better performance than the BSL model when predicting flow separation with adverse
pressure gradients. Blending is handled the same way as in the BSL model.

\[ \mu_t = \frac{\bar{p} a_1 k}{\max (a_1 \omega, \Omega F_2)} \quad (2.83) \]

\[ F_2 = \tanh(\text{arg}_2^2) \quad (2.84) \]

\[ \text{arg}_2 = \max \left[ \frac{2 \sqrt{k}}{0.09 \omega_d}, \frac{500 \nu}{d^2 \omega} \right] \quad (2.85) \]

\[ a_1 = 0.31 \quad (2.86) \]
Chapter 3

Numerical Methods

3.1 Numerical Formulation

In order to solve the RANS or LES equations in finite locations in space and time, the time and spatial derivatives must be discretized. The discretized equations must be evaluated and solved using a time-integration technique. This chapter will discuss the techniques used in the REACTMB solver for discretizing and solving the compressible reactive Navier-Stokes equations. Methods for improving the accuracy of the solution will also be discussed. First, the equations must be written in vector form as shown in Eq. 3.1, where \( \mathbf{U} \) is the vector of conserved variables, \( \mathbf{F} \) is the vector of inviscid fluxes, \( \mathbf{G} \) is the viscous flux, and \( \mathbf{S} \) is the source vector.

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_j}{\partial x_j} + \frac{\partial \mathbf{G}_j}{\partial x_j} = \mathbf{S}
\]  

(3.1)

These vectors are defined as follows.

\[
\mathbf{U} = \begin{bmatrix}
\overline{\rho}_1 \\
\vdots \\
\overline{\rho}_N \gamma \\
\overline{\rho}
\end{bmatrix}
\]  

(3.2)
Discretization of Eq. 3.1 can be achieved using a variety of methods; REACTMB uses a finite-volume approach to perform the discretization. The finite-volume formulation involves discretizing the equations over a finite number of small volumes and integrating the equation over the control volume (CV) defined by the cell.

\[
\int_{CV} \frac{\partial U}{\partial t} \, dV + \int_{CV} \frac{\partial F_j}{\partial x_j} \, dV + \int_{CV} \frac{\partial G_j}{\partial x_j} \, dV = \int_{CV} S \, dV
\]  

(3.6)
The Green-Gauss (or divergence) theorem, as shown in Eq. 3.7, is used to equate the volume integrals into surface integrals over the control surface (CS) defining the cell volume.

\[
\int_{CV} \frac{\partial T_{ijk}}{\partial x_i} dV = \int_{CS} n_i T_{ijk} dS \tag{3.7}
\]

Applying Eq. 3.7 to the flux derivatives in Eq. 3.6 results in the equation below.

\[
\int_{CV} \frac{\partial U}{\partial t} dV + \int_{CS} n_j F_j dS + \int_{CS} n_j G_j dS = \int_{CV} S dV \tag{3.8}
\]

Now the integrals can be evaluated with discrete approximations as shown in Eq. 3.9, where \( NF \) is the number of faces defining a cell, \( A_f \) is the face area, and \( V_{CV} \) is the cell volume. The time derivative is approximated by the change in the conservative variables, \( \Delta U \), for a given time step \( \Delta t \).

\[
\frac{\Delta U}{\Delta t} V_{CV} + \sum_{f=1}^{NF} (n_j F_j)_f A_f + \sum_{f=1}^{NF} (n_j G_j)_f A_f = S V_{CV} \tag{3.9}
\]

One advantage of the finite volume approach is that it is physically intuitive. The change in a variable within a cell volume is equal to the summation of the fluxes through the cell faces. These flux terms are evaluated by the projection of the flux vectors along the normal vector of the face. Also, we recognize that the normal vector to one cell’s face is equal and opposite to the adjacent cell. This implies that the summation of all of the fluxes through the internal domain will equal zero, enforcing the important conservation requirement. However, these equations are not quite capable of properly capturing the physics of compressible flows. An issue in compressible flows involves the propagation of information and its relation to the speed of sound. This requires some special consideration as described in the following section.

### 3.2 Upwinding and Flux-Vector Splitting

For the compressible Navier-Stokes equations, the classification of the inviscid fluxes can change based on Mach number. For subsonic flows the spatial fluxes are elliptic, meaning that properties in the flow at an individual point is dependent on the properties everywhere else in the flow. However, when transitioning to the supersonic regime, the equations become hyperbolic. In order to understand this, we consider the propagation of information through a 1D flow in the form of characteristic waves. In the case of subsonic flows, the fluid either does not move or moves more slowly than the speed of the characteristic waves. These characteristic waves move at the local speed of sound, relative to the particle. The fact that these waves move with the speed of sound relative to the particle is very important. If the particle is not moving (or moving with a slow speed) the propagation of information due to a disturbance moves at the
speed of sound in both directions. Now if we consider a particle that is already moving at the speed of sound, the wave of information cannot move in the opposite direction of the motion of the particle, and can only move in the direction of the particle’s motion. To clarify this, the speed, and direction, at which information travels due to disturbances is defined below.

\begin{align}
  c^+ &= u + a \\  c^- &= u - a
\end{align}  \hspace{1cm} (3.10)

Here, ‘+’ denotes the right and ‘-’ denotes the left, where \( c \) is the characteristic wave speed, \( u \) is the particle speed, and \( a \) is the local speed of sound. So for a particle moving from left to right at a speed greater than Mach 1, the characteristic wave speed to the left and right will both be positive (to the right). This means that in a supersonic flow, the properties of a particle is only dependent on information ‘upwind’ of the flow, or in other words, information only travels ‘downwind.’

In the finite volume formulation, the inviscid flux vector is the expression for the transmission of this information throughout the flow field. In order to properly capture the physics at all speeds, the local Mach number must be taken into account. One method for doing this is called flux-vector splitting. This method splits the inviscid flux vector into the ‘upwind’ and ‘downwind’ components. As the local normal Mach number exceeds one, the downwind contribution goes to zero and the scheme becomes a pure ‘upwinding’ method. For normal Mach numbers less than one, the flux-splitting method includes both the ‘upwind’ and ‘downwind’ portions of the flux. It is noted that the viscous fluxes are discretized using a second order central finite difference method regardless of Mach number.

The flux-splitting scheme used in this work is the low-diffusion flux-splitting scheme (LDFSS), which was developed by Edwards [25] as a variant of the standard Van Leer scheme. The LDFSS scheme decomposes the face-normal projection of the inviscid flux vector into convective and pressure components. These components are defined in Eq. 3.13.

\[ n_j F_j = (n_j F_j)^c + (n_j F_j)^p = \bar{\rho} n_j \bar{u}_j E^c + \bar{\rho} E^p \]  \hspace{1cm} (3.12)
The flux splitting is determined at a cell face positioned between cells \( i \) and \( i + 1 \), named face \( i + 1/2 \). The splitting is performed based on the information at the left (L) and right (R) sides of the face. After the splitting, the convective component is expressed as shown, where \( a \) refers to the sound speed.

\[
(n_j \mathbf{F}_j)_{i+1/2}^c = a_{i+1/2} \left[ \mathbf{p}_L C^+ \mathbf{E}_L^c + \mathbf{p}_R C^- \mathbf{E}_R^c \right]
\]

(3.14)

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

(3.15)

\[
C^+ = \alpha_L^+ (1 + \beta_L) M_L - \beta_L M_L^+ - M_{1/2}^+
\]

(3.16)

\[
C^- = \alpha_R^+ (1 + \beta_R) M_R - \beta_R M_R^+ + M_{1/2}^-
\]

(3.17)

\[
M_{1/2}^+ = M_{1/2} \left[ \frac{2\mathbf{p}_R}{\mathbf{p}_R + \mathbf{p}_L} - \delta \frac{|\mathbf{p}_L - \mathbf{p}_R|}{\mathbf{p}_L} \right], \quad \delta = 2.0
\]

(3.18)

\[
M_{1/2}^- = M_{1/2} \left[ \frac{2\mathbf{p}_L}{\mathbf{p}_R + \mathbf{p}_L} - \delta \frac{|\mathbf{p}_L - \mathbf{p}_R|}{\mathbf{p}_R} \right], \quad \delta = 2.0
\]

(3.19)

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

(3.20)

\[
\beta_{L/R} = - \max \left[ 0, 1 - \text{int}(|M_{L/R}|) \right]
\]

(3.21)

\[
M_{L/R}^\pm = \pm \frac{1}{4} \left[ |M_{L/R} \pm 1| \right]^2
\]

(3.22)

\[
M_{1/2} = \frac{1}{2} \beta_L \beta_R \left[ \sqrt{\frac{1}{2} (M_L^2 + M_R^2)} - 1 \right]
\]

(3.23)

\[
M_{L/R} = \frac{n_j \bar{u}_{jL/R}}{a_{i+1/2}}
\]

(3.24)

The pressure component is split according to the following equations.

\[
(n_j \mathbf{F}_j)_{i+1/2}^p = \mathbf{E}_{i+1/2}^p \left[ D^+_L \mathbf{p}_L + D^+_R \mathbf{p}_R \right]
\]

(3.25)
\[ D_{L/R}^\pm = \alpha_{L/R}^\pm [1 + \beta_{L/R}] - \beta_{L/R} p_{L/R}^\pm \] (3.26)

\[ p_{L/R}^\pm = \frac{1}{4} (M_{L/R} \pm 1)^2 (2 \mp M_{L/R}) \] (3.27)

The standard approximation of the (L) and (R) components is simply the cell-centered data from cells \( i \) and \( i + 1 \), respectively. This is the first-order numerical scheme for the inviscid flux. An extension to higher-order accuracy is beneficial for better capturing of shocks and discontinuities. Methods for higher-order extension are explained in the next section.

### 3.3 Higher-Order Extension

In order to increase the order of accuracy of the solution, several methods are employed into REACTMB. Increased spatial accuracy can be achieved by implementing methods for reconstructing the interface values in the inviscid flux calculation. Methods that preserve monotonicity such as the Total Variation Diminishing (TVD) scheme can be used to reconstruct the primitive variables to the interface [58]. These methods excel at capturing discontinuities (such as shocks) without introducing oscillations. However, this method can be quite dissipative. This isn’t always desirable in areas where oscillatory behavior due to turbulence is physically accurate. Thus REACTMB includes options for a less dissipative method in the Piecewise Parabolic Method (PPM) [59] as well as the option of using the Ducros switch [60], which shifts to a fourth-order central difference scheme in the areas of high vorticity. An Essentially Non-Oscillatory Piecewise Parabolic Method (ENO-PPM) [61] is also available as an alternative to the Ducros switch for low-speed flows. These methods are discussed in the following sub-sections.

#### 3.3.1 Total Variation Diminishing (TVD) Method

The first method for reconstructing the primitive variables to the interface between cells is the total variation diminishing (TVD) approach [58]. The vector of primitive variables, required for this method, is given below.

\[ \bar{V} = \begin{bmatrix}
\bar{p}_1 \\
\vdots \\
\bar{p}_{NS} \\
\bar{u}_1 \\
\bar{u}_2 \\
\bar{u}_3 \\
\bar{T} \\
k \\
\omega
\end{bmatrix}, \quad \bar{p}_s = \bar{p}_j R_s T \] (3.28)
The left and right states are determined using a ‘minmod’ function for the interface $i + 1/2$ as shown below.

\[ V_{L,i+1/2} = V_i + \frac{1}{2} \minmod(V_{i+1} - V_i, V_i - V_{i-1}) \] (3.29)

\[ V_{R,i+1/2} = V_{i+1} - \frac{1}{2} \minmod(V_{i+2} - V_{i+1}, V_{i+1} - V_i) \] (3.30)

\[ \minmod(a, b) = \begin{cases} 
  a & \text{if } |a| < |b| \text{ and } ab > 0 \\
  b & \text{if } |b| < |a| \text{ and } ab > 0 \\
  0 & \text{if } ab \leq 0 
\end{cases} \] (3.31)

3.3.2 Piecewise Parabolic Method (PPM)

The next option for extending the order of accuracy is the PPM scheme as given in [59]. This method first requires determining initial left and right states using a fourth order central difference, as shown below.

\[ V_{L,i+1/2} = V_{R,i+1/2} = \frac{7}{12} (V_i + V_{i+1}) - \frac{1}{12} (V_{i+2} + V_{i-1}) \] (3.32)

This value will normally be assigned as the left and right values of the primitive variables at the interface. However, there are some cases where this would lead to an interpolation which leads to values outside of the range between the left and right cell data. To preserve the monotonicity of the function, the following definitions are used, where the expressions for the parameters $C$ and $D$ are defined in Eqns. 3.35 and 3.36.

\[ V_{L,i+1/2} = \begin{cases} 
  V_i & \text{if } (V_{R,i-1/2} - V_i)(V_i - V_{L,i+1/2}) \leq 0 \\
  3V_i - 2V_{R,i-1/2} & \text{if } -C \times C > D \times C \\
  V_{L,i+1/2} & \text{else} 
\end{cases} \] (3.33)

\[ V_{R,i-1/2} = \begin{cases} 
  V_i & \text{if } (V_{R,i-1/2} - V_i)(V_i - V_{L,i+1/2}) \leq 0 \\
  3V_i - 2V_{L,i+1/2} & \text{if } D \times C > C \times C \\
  V_{R,i-1/2} & \text{else} 
\end{cases} \] (3.34)

\[ C = (V_{L,i+1/2} - V_{R,i-1/2}) \] (3.35)

\[ D = 6 \left( V_i - \frac{1}{2} (V_{L,i+1/2} + V_{R,i-1/2}) \right) \] (3.36)

This method enforces monotonicity while adding some degree of dissipation proportional to the difference between the initial and final states. As was the case for the TVD method, this makes this method good for capturing shocks, but is not ideal for locations where turbulence causes oscillations. To address this, for both PPM and TVD, the Ducros switch is implemented.
3.3.3 Ducros Switch

As mentioned before, in highly turbulent flows it is desirable to preserve some of the oscillatory behavior when using LES techniques. REACTMB uses the blending function developed by Ducros et al. [60] to blend the monotonic reconstruction with the fourth-order central difference reconstruction. This allows for the monotonicity preserving methods to be used near shocks and the fourth-order central difference to be used in vorticity dominated regions. The blending function is defined by Eq. 3.37, where $\mathbf{u}$ is the velocity vector and $\varepsilon$ is a small constant to avoid division by zero.

$$\Gamma^D = \frac{(\nabla \cdot \mathbf{u})^2}{(\nabla \cdot \mathbf{u})^2 + |\nabla \times \mathbf{u}|^2 + \varepsilon_i^2}, \quad \varepsilon_i = \frac{1 \times 10^{-8} U_\infty}{\max(\Delta x, \Delta y, \Delta z)_i}$$ (3.37)

This function approaches zero in weakly compressible, turbulent regions while going to one in shock-dominated regions. The reconstructed cell interface values are given by Eqns. 3.38 and 3.39 where $V^M$ denotes the monotonicity preserving reconstruction (using TVD or PPM) and $V^C$ is the central difference reconstruction given by Eq. 3.32.

$$V_{L,i+1/2} = (1 - \Gamma^D)_i V^C_{i+1/2} + \Gamma^D V^M_{L,i+1/2}$$ (3.38)

$$V_{R,i+1/2} = (1 - \Gamma^D)_{i+1} V^C_{i+1/2} + \Gamma^D V^M_{R,i+1/2}$$ (3.39)

Once the primitive variables are determined, they are used to calculate the conservative variable inviscid flux vector. The LDFSS method only describes the inviscid portion of the fluxes. The viscous portion does not require splitting, and is discretized using a second-order central difference method.

3.3.4 Essentially Non-Oscillatory Piecewise Parabolic Method (ENO-PPM)

An alternative method to the Ducros switch was implemented for low-speed flow simulations. An Essentially Non-Oscillatory version of the PPM scheme is used to blend the fourth-order central difference, $V^C_{i+1/2}$, with PPM. This scheme is defined by Eq. 3.40. Note that $V^M_{L/R,i+1/2}$ is the vector of primitive variables obtained from the PPM scheme. The difference between this scheme and the Ducros switch is that it is performed on a per-variable basis, and it is purely mathematical.

$$V_{L,i+1/2} = V^C_{i+1/2} + \Gamma^\text{ENO}_i \left( V^M_{L,i+1/2} - V^C_{i+1/2} \right)$$

$$V_{R,i+1/2} = V^C_{i+1/2} + \Gamma^\text{ENO}_{i+1} \left( V^M_{R,i+1/2} - V^C_{i+1/2} \right)$$ (3.40)

$$\Gamma^\text{ENO}_i = \left( \frac{|V_{i+1} - V_i| - |V_i - V_{i-1}|}{|V_{i+1} - V_i| + |V_i - V_{i-1}| + \varepsilon} \right)$$ (3.41)
3.4 Time Integration

Given equations to determine the flux and source terms for a given time step, it is possible to update the solution in time to obtain a time-accurate simulation over the domain. While it is relatively simple to solve for \( \Delta U / \Delta t \) explicitly, the limitations of the time step make it impractical. To reduce the cost of these simulations a more stable, implicit method is required. The REACTMB code uses the implicit Crank-Nicolson time integration procedure to solve this problem. Unlike explicit methods, the implicit method makes use of information from the subsequent time-steps to iteratively solve for the solution at the next physical time step. In order to apply an update procedure, we must first formulate the linearized system.

The current method first takes the discretized governing equations, Eq. 3.9 and recasts them into contributions from the orthogonal face directions (i,j, and k terms). This method requires a structured mesh that consists of hexahedral cells with distinct i,j, and k directions. Note that the inviscid and viscous fluxes have combined into a vector \( \mathbf{E} \) here. Further, recall that the quantity \( (\mathbf{E}_j n_j)_f \) represents normal projection of the flux passing through the cell face, \( f \).

\[
\mathbf{E}_j = \mathbf{F}_j + \mathbf{G}_j
\]

\[
\frac{\Delta U}{\Delta t} \nabla_{CV} + \sum_{i\text{-face}} (\mathbf{E}_j n_j)_f A_f + \sum_{j\text{-face}} (\mathbf{E}_j n_j)_f A_f + \sum_{k\text{-face}} (\mathbf{E}_j n_j)_f A_f = SV_{CV} \tag{3.42}
\]

The residual vector is defined as the sum of all the fluxes and source terms as defined below.

\[
\mathbf{R} = \sum_{i\text{-face}} (\mathbf{E}_j n_j)_f A_f + \sum_{j\text{-face}} (\mathbf{E}_j n_j)_f A_f + \sum_{k\text{-face}} (\mathbf{E}_j n_j)_f A_f - SV_{CV} \tag{3.43}
\]

This expression can be re-written in terms of the fluxes at the interfaces of cells. The interface fluxes are defined as shown in Eq. 3.44.

\[
\begin{align*}
\mathbf{E}_{i+\frac{1}{2}} & \equiv (\mathbf{E}_j n_j)_{i+\frac{1}{2},j,k} A_{i+\frac{1}{2},j,k} \\
\mathbf{E}_{j+\frac{1}{2}} & \equiv (\mathbf{E}_j n_j)_{i,j+\frac{1}{2},k} A_{i,j+\frac{1}{2},k} \\
\mathbf{E}_{k+\frac{1}{2}} & \equiv (\mathbf{E}_j n_j)_{i,j,k+\frac{1}{2}} A_{i,j,k+\frac{1}{2}}
\end{align*} \tag{3.44}
\]

By careful inspection, it is noted that the cell-specific interface fluxes are equal and opposite between two adjacent cells. This fact can be used to simplify storage and calculation of the interface fluxes. Using this simplification, the expressions in 3.44 are substituted into Eq. 3.43 to provide the expression for the steady-state residual vector, \( \mathbf{R}_s \).

\[
\mathbf{R}_s = \left( \mathbf{E}_{i+1/2} - \mathbf{E}_{i-1/2} \right) + \left( \mathbf{E}_{j+1/2} - \mathbf{E}_{j-1/2} \right) + \left( \mathbf{E}_{k+1/2} - \mathbf{E}_{k-1/2} \right) - SV_{CV} \tag{3.45}
\]
This steady residual can be calculated using the field of primitive variables at the current time step, \( V_n \). The implicit Crank-Nicholson scheme involves the calculation of an unsteady residual as shown in Eq. 3.46 based on the field of variables at the current time step and the next time step.

\[
R_n^{n+1} = V_{CV} \frac{U_n^{n+1} - U_n^n}{\Delta t} + \frac{1}{2} \left[ R_s \left( V_n^{n+1} \right) + R_s \left( V_n^n \right) \right] = 0 \quad (3.46)
\]

Obviously, the primitive variables at the next time step are not known, thus a sub-iterative procedure is required that will eventually converge to the next time level. This sub-iteration will be denoted by the \( k \) superscript. Substituting Eq. 3.45 into Eq. 3.46 and using the sub-iterative notation yields Eq. 3.47.

\[
V_{CV} \frac{U_n^{n+1,k+1} - U_n^n}{\Delta t} + \frac{1}{2} \left[ \left( E_{i+1/2} - E_{i-1/2} \right)^{n+1,k+1} + \left( E_{i+1/2} - E_{i-1/2} \right)^n \right] \\
+ \frac{1}{2} \left[ \left( E_{j+1/2} - E_{j-1/2} \right)^{n+1,k+1} + \left( E_{j+1/2} - E_{j-1/2} \right)^n \right] \\
+ \frac{1}{2} \left[ \left( E_{k+1/2} - E_{k-1/2} \right)^{n+1,k+1} + \left( E_{k+1/2} - E_{k-1/2} \right)^n \right] \\
+ \frac{1}{2} \left[ \left( -S_{n+1,k+1} - S_n \right) V_{CV} \right] = R_n^{n+1,k+1} = 0 \quad (3.47)
\]

The next step is to relate the fluxes at the next sub-iterative time step to the data at the current time level. This is done by linearizing these terms using a first-order Taylor series expansion in pseudo-time as shown below where the change in the primitive variable vector in pseudo-time is defined as well.

\[
E_{(i,j,k) \pm \frac{1}{2}}^{n+1,k+1} = E_{(i,j,k) \pm \frac{1}{2}}^{n+1,k} + \left( \frac{\partial E}{\partial V} \right)^n_{(i,j,k) \pm \frac{1}{2}} \Delta V_{(i,j,k) \pm \frac{1}{2}}^{n+1,k} \quad (3.48)
\]

\[
\Delta V_{n+1,k} = V_{n+1,k+1} - V_{n+1,k} \quad (3.49)
\]

The term \( \left( \frac{\partial E}{\partial V} \right) \) is the flux Jacobian matrix and determines the partial derivatives of the fluxes with respect to the primitive variables. Because the fluxes are determined at the flux interfaces, the flux Jacobian must be split for each cell interface with respect to the cell-centered variables. The splitting of the flux
Jacobian is defined in Eq. 3.50 while the elements $A^\pm - F^\pm$ are given in Eq. 3.51.

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

\[
A^+ = \frac{\partial E_{i+1/2}}{\partial V_{i,j,k}} \quad A^- = \frac{\partial E_{i+1/2}}{\partial V_{i+1,j,k}}
\]
\[
B^+ = \frac{\partial E_{i-1/2}}{\partial V_{i,j,k}} \quad B^- = \frac{\partial E_{i-1/2}}{\partial V_{i,j,k}}
\]
\[
C^+ = \frac{\partial E_{j+1/2}}{\partial V_{i,j,k}} \quad C^- = \frac{\partial E_{j+1/2}}{\partial V_{i,j+1,k}}
\]
\[
D^+ = \frac{\partial E_{j-1/2}}{\partial V_{i,j+1,k}} \quad D^- = \frac{\partial E_{j-1/2}}{\partial V_{i,j+1,k}}
\]
\[
E^+ = \frac{\partial E_{k+1/2}}{\partial V_{i,j,k}} \quad E^- = \frac{\partial E_{k+1/2}}{\partial V_{i,j,k+1}}
\]
\[
F^+ = \frac{\partial E_{k-1/2}}{\partial V_{i,j,k}} \quad F^- = \frac{\partial E_{k-1/2}}{\partial V_{i,j,k}}
\]

The Jacobians of the conservative variable vector and source term vector are linearized in a similar fashion as shown below.

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

Eqns. 3.48 - 3.54 can be substituted into Eq. 3.47 to derive the unsteady residual equation in terms
of the Jacobians and the change in the primitive variables for each sub-iteration.

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

(3.55)

Eq. 3.55 represents a linear system of equations over the space of all of the cells within the computational domain. The linear system can be expressed in the usual \(Ax = b\) form as shown in Eq. 3.56.

\[
A \Delta V^{n+1,k} = -R_{u}^{n+1,k}
\]

(3.56)

With this discretization, \(A\) is a sparse matrix with seven diagonals and \(\Delta V^{n+1,k}\) is the correction vector for the primitive variables at every sub-iteration. The system can be solved using many different methods; the method used in these studies is the incomplete lower-upper (ILU) factorization method. Once the system in Eq. 3.56 is solved for the correction vector, Eq. 3.57 is used to update the flow solution for each sub-iteration.

\[
V^{n+1,k+1} = V^{n+1,k} + \Delta V^{n+1,k}
\]

(3.57)

The solution at the next physical time step is taken to be the solution at the last sub-iteration.

\[
V^{n+1} = V^{n+1,k_{max}}
\]

(3.58)

Usually the maximum number of sub-iterations is set to 6 or 7. The sub-iterations are also monitored for convergence. If the unsteady residual magnitude is decreased to a sufficiently small magnitude relative to the initial value, the sub-iterations are taken to be converged and the solution is updated. The updated primitive variables are then used to re-compute the fluxes, conserved variables, source terms, and Jacobians as the cycle continues.
Chapter 4

Combustion Closure Models

In this chapter, we will briefly review turbulent combustion models that are available in the literature, and define the closure models implemented in this study. Combustion closure models are required to provide an expression for the filtered source term in the LES species continuity equations (Eq. 2.59). The focus of this research is on LES closure modeling, so the models referred to here are directed to LES rather than RANS modeling. Details for models related to the type of closure we are developing will be discussed first and in more detail. The form of our closure resembles that of a thickened flame model and incorporates ideas similar to scale-similarity and Partially Stirred Reactor (PaSR) models. PDF based, deconvolution, and ODT methods are also summarized for a more complete discussion of the closure models that are available. At the end of this chapter, previous models developed by our group are summarized, and the new family of models are defined. For further reading on different closure models, for both RANS and LES, refer to [62] and [63].

4.1 Laminar Chemistry

The simplest and most basic form of closure for the filtered species source term, based on finite rate chemistry, is that provided by the laminar chemistry. This is the state of the practice for high-speed combustion due to its simplicity. The source terms can be calculated based on the law of mass action as given by Eq. 4.1. The net reaction rate can be determined by Eq. 4.2, where the rate coefficient can be determined by an Arrhenius form. The parameters for the Arrhenius equation are given by reduced reaction mechanisms. The filtered source term is simply taken to be equal to the source terms based on the resolved flow variables. This model is named ‘laminar chemistry,’ because it neglects the effect of
subgrid fluctuations in species densities and temperatures entirely.

\[
\dot{\omega}_s(\rho_s, T) = M_w, s \sum_{k=1}^{NR} (v''_{s,k} - v'_{s,k}) R_k
\]  

(4.1)

\[
R_k = k_{f,k} \prod_{s=1}^{NS} \left( \frac{\rho_s}{M_{w,s}} \right)^{\nu'_{s,k}} - k_{b,k} \prod_{s=1}^{NS} \left( \frac{\rho_s}{M_{w,s}} \right)^{\nu''_{s,k}}
\]  

(4.2)

\[
\bar{\omega}_k(\rho_s, T) = \omega_k(\bar{\rho}_s, \bar{T})
\]  

(4.3)

### 4.2 Thickened Flame Models

One problem that arises in LES of premixed flames is that the flame thickness is on the order of a millimeter and can be smaller than the LES mesh size. A simple closure model that is directly aimed at attempting to help solve this issue is the thickened flame model (TFM). The basic idea is to consider a flame thicker than the actual one but retaining the same laminar flame speed. Laminar flame speeds and thicknesses can be related to diffusivity and mean reaction rates. The flame can be thickened by scaling the diffusivity up by some thickening factor, and scaling the reactivity down by the same factor. This means that the same laminar flame speed is maintained while increasing the flame thickness by a factor, \( F \). Therefore, for sufficiently large \( F \), the flame can be resolved for a given mesh scale and additional models may be used to account for subgrid scale effects. \( F \) is normally chosen based on the number of grid points desired to resolve the flame front (typically 4-10). An approximation for the required \( F \) based on approximate laminar flame thickness and mesh scale is given by Eq. 4.4. One drawback of this method, is that the flame response is modified by the thickening especially for very high turbulence levels. The Damköhler number, as defined in Eq. 4.5, is also scaled down by the factor \( F \) [64]. Note that \( \tau_m \) and \( \tau_c \) are turbulent mixing and chemical time scales, respectively. The adjusted molecular diffusivity is given by Eq. 4.6, and the basic thickened flame model is given by Eq. 4.7. Note that the thickened flame model only attenuates reactivity.

\[
F = \frac{nA}{\delta_f}
\]  

(4.4)

\[
D_a = \frac{\tau_m}{\tau_c}
\]  

(4.5)

\[
D_{TFM} = FD
\]  

(4.6)

\[
\bar{\omega}_k(\rho_s, T) = \frac{\alpha_k(\bar{\rho}_s, \bar{T})}{F}
\]  

(4.7)

The model above is very simple in that it uses a constant \( F \) and does not incorporate subgrid scale effects. In [65], subgrid scale effects were incorporated by estimating the flame wrinkling factor \( \Xi \). This
is the ratio of turbulent to laminar flame speeds or total flame area to projected area. A correction for the flame wrinkling effect is required as the thickened flame will underestimate the wrinkling due to turbulent fluctuations compared to the actual flame. This is also represented by the fact that the standard TFM scales down the Damköhler number. The adjusted source term for the thickened flame model with subgrid scale is given by Eq. 4.8, where Ξ is a function of the grid scale, laminar flame speed and thickness, $rms$ velocity and Reynolds number as shown in Eq. 4.9. In Eq. 4.9, $\Gamma$ is an effective straining function that is designed to account for all relevant scales based on DNS results. For the adjusted model, the diffusivity is also scaled by the flame wrinkling factor, resulting in a flame of thickness $F\delta_l^o$ and a speed $\Xi s_l^o$, which should be closer to the turbulent flame speed. A dynamic model for the flame wrinkling factor is presented in [66].

$$\frac{\omega_l(\rho_s, T)}{F} = \Xi \frac{\omega_l(\bar{\rho}_s, \bar{T})}{F}$$

$$\Xi \left( \frac{\Delta}{\delta_l^o}, \frac{u_A^l}{s_l^o}, Re_\Delta \right) = \left( 1 + \min \left[ \frac{\Delta}{\delta_l^o}, \Gamma \frac{U_A^l}{s_l^o} \right] \right)^\beta$$

$$D_{TFM} = \Xi FD$$

The flame wrinkling factor can be used to provide closure to the filtered chemical source terms without thickening of the flame as well. The generic form for the filtered reaction rate based on the flame wrinkling model is given in Eq. 4.11. This model requires closure of $\Xi$ in order to estimate the ratio of total to resolved flame surfaces in the filtered volume. In short, if the resolved is equal to the actual flame surfaces, $\Xi = 1$, and the laminar flame assumption holds. However, if the total flame surfaces are greater or less than the resolved flame surfaces, due to turbulent fluctuations, $\Xi$ should be modeled to account for these effects accordingly. A description and analysis of several different dynamic models for the flame wrinkling factor are given in [67]. It should also be mentioned that a limitation to the thickened-flame method is that there is no direct extension to non-premixed or partially premixed flames.

$$\frac{\omega_l(\rho_s, T)}{F} = \Xi \omega_l(\bar{\rho}_s, \bar{T})$$

### 4.3 Partially Stirred Reactor Model

The laminar chemistry model implies that the mixture of gases reacting in a cell volume are perfectly mixed, thus the use of the filtered mean variables in determining chemical source terms. The Partially Stirred Reactor (PaSR) model attempts to correct for the reactivity by modeling the volume fraction of the parts that are and are not reacting. This can be done by proposing equations that divide a cell into fine and surrounding structures as described by Berglund, et al [68]. The mixing and reactions are assumed to take place in the fine structures (*) while the surroundings are dominated by large-scale
coherent flow structures ($^o$). These two parts are combined to equal the resolved quantity, $\psi$, as shown in Eq. 4.12. Sabelnikov and Fureby derive their Extended-PaSR model in [69]. Considering only the species equations, the fine and surrounding structures must obey the equations given by Eqns. 4.13 and 4.14, respectively. Note that $\gamma$ is denoting the fine and surround volume fractions.

$$\tilde{\psi} = \gamma \psi^o + (1 - \gamma) \psi^e$$  \hspace{1cm} (4.12)

$$\partial_t (\gamma^o \rho^o_s) + \nabla \cdot (\gamma^o \rho^o_s v^o) = \nabla \cdot (\gamma^o (k_s - b_s)) + \gamma^o \bar{\omega}_s^o + \bar{M}_s^o$$  \hspace{1cm} (4.13)

$$\partial_t (\gamma^e \rho^e_s) + \nabla \cdot (\gamma^e \rho^e_s v^e) = \nabla \cdot (\gamma^e (k_s - b_s)) + \gamma^e \bar{\omega}_s^o + \bar{M}_s^o$$  \hspace{1cm} (4.14)

Here $k_s$ and $b_s$ are the diffusive and subgrid scale transport terms, respectively. $M_s$ is the exchange term between the fine and surrounding structures.

Equations 4.13 and 4.14 can be solved together for the fine and surrounding parts and then recombined to for the resolved quantity from $\tilde{\rho}_s = \gamma^o \rho^o_s + (1 - \gamma^o) \rho^e_s$. A more convenient approach is to solve the balance equations for the fine structure fractions along with the LES balance equation given by Eq. 4.15, once $\gamma^o$, $M_s^o$, and a relationship between $\bar{\omega}_s$ and $\bar{\omega}_s^o$ are provided.

$$\partial_t (\tilde{\rho}_s) + \nabla \cdot (\tilde{\rho}_s \tilde{v}) = \nabla \cdot (\gamma^o (k_s - b_s)) + \gamma^o \bar{\omega}_s^o + \bar{M}_s$$  \hspace{1cm} (4.15)

Based on the relationship between the fine, surrounding and resolved quantities and the nature of the transport equations, the filtered chemical source term can be defined as $\tilde{\rho}_s = \gamma^o \tilde{\rho}_s^o + (1 - \gamma^o) \tilde{\rho}_s^e$. However, most observations leads to the assumption that most of the exothermal reactions occur in the fine structures [68]. So, the filtered reaction rate can be estimated by $\tilde{\omega}_s \approx \gamma^o \tilde{\omega}_s^o$. The exchange term is modeled as shown in Eq. 4.16, where the mass rate of change between the fine and surrounding structures is given by Eq. 4.17.

$$\bar{M}_s^o = \frac{1}{2} (\dot{m} + |\dot{m}|) Y_s^o + \frac{1}{2} (\dot{m} + |\dot{m}|) Y_s^o - \frac{\gamma^o \bar{\rho}(Y_s^o - \bar{Y}_s)}{\tau (1 - \gamma^o)}$$  \hspace{1cm} (4.16)

$$\dot{m} = -\frac{\bar{\rho}(\gamma^o - \gamma_{eq})}{\tau^o}$$  \hspace{1cm} (4.17)

Thus, the extended PaSR model can be summarized by the governing equations for reactive species given by Eq. 4.18, along with LES filtered momentum and energy equations. The model requires solving the filtered species continuity, momentum and energy equations. The fine structures are evaluated by
solving 4.14 with the source term being evaluated for the fine structure conditions \( \omega_s = \bar{\omega}_s(Y_s^*, T^*) \).

\[
\partial_t(\tilde{\rho}_s) + \nabla \cdot (\tilde{\rho}_s \tilde{v}) = \nabla \cdot (k_s - b_s) + \bar{\omega}_s
\]

\[
\partial_t(\gamma^s \rho_s) + \nabla \cdot (\gamma^s \rho_s \tilde{v}) = \nabla \cdot (\gamma^s (k_s - b_s)) + \gamma^s \bar{\omega}_s + \bar{M}_s
\]

\[
\bar{\omega}_s = \gamma^s \bar{\omega}_s^s
\]

(4.18)

Closure remains for the equilibrium fine-structure volume fraction and fine-structure residence time \( \gamma_{eq}^s \) and \( \tau^s \), respectively. These are given by Eqns. 4.19 and 4.20.

\[
\tau^s = \sqrt{\tau_K \tau_D}
\]

(4.19)

\[
\gamma_{eq}^s = \frac{\tau_c}{\tau_m + \tau^s}
\]

(4.20)

By neglecting subgrid convection, a simpler PaSR model can be derived [68]. This is summarized by Eqns. 4.21 and 4.22 which define the subgrid balance equations that couple the fine and surrounding structures for mass and energy, respectively. In these equations, \( \tau_m \) is the subgrid mixing time while \( \gamma \) is the reacting volume fraction. These both require estimation based on the resolved scales in order to complete the subgrid model.

\[
\bar{\rho}(Y_s^* - \bar{Y}_s) = (1 - \gamma) \tau_m \bar{\omega}_s(\bar{\rho}, Y_s^*, T^*)
\]

(4.21)

\[
\bar{\rho} \sum_{s=1}^{NS} [Y_s^* h_s^s(T^*) - \bar{Y}_s h_s^s(\bar{T})] = (1 - \gamma) \tau_m \sum_{s=1}^{NS} h_s^0 \bar{\omega}_s(\bar{\rho}, Y_s^*, T^*)
\]

(4.22)

According to [68] the mixing time scale can be approximated as the harmonic mean of the Kolmogorov and integral length scales \( \tau_m = \sqrt{\tau_K T} \), while \( \gamma \) can be estimated as the ratio of the volumes swept by the reacting structures to the combined volume of the reacting and mixing structures so that \( \gamma = \tau_c / (\tau_m + \tau_c) \). The simplest PaSR type model can then be defined as shown in Eq. 4.23. Note that \( \tau_c \) is the chemical time scale which is should be defined to be representative of the overall chemical reaction. For premixed flames, the definition given by 4.24 can be used, where \( \delta_l \) and \( s_l \) are the laminar flame thickness and speed, respectively. An alternative definition is given by 4.25, where the chemical time scale is defined as the ratio of mixture density to overall reactivity.

\[
\bar{\omega}_s(\rho_s, T) = \frac{\tau_c}{\tau_m + \tau_c} \bar{\omega}_s(\rho_s, T)
\]

(4.23)

\[
\tau_c \approx \frac{\delta_l}{s_l}
\]

(4.24)
Inspecting the models, some simple conclusions can be drawn. This model only allows for attenuation of the fine-structure’s source terms. Although this does not guarantee that this model will diminish reactivity relative to laminar chemistry, it is highly likely. This is based on the assumption that the majority of the exothermal reactions occur within the fine structures. A general theme in these types of closures is the incorporation of chemical and mixing time scales in defining the model. The Extended-PaSR model (Eqn. 4.18) is much more complex than the simplified PaSR model (Eq. 4.23) or TFM in that it adds an additional set of species and energy-conservation equations for the fine-scale properties.

### 4.4 Scale-Similarity Based Models

Scale-similarity type models usually attempt to model the filtered chemical source term by breaking it into the resolved and subgrid scale components using variations of the Germano identity [70]. Many variations of these types of methods exist. In [70], many applications are described for which the Germano identity is useful in modeling, including subgrid-scale flux calculations and modeling of reaction rates. A general additive form for subgrid closure modeling is shown in Eq. 4.26 while the multiplicative form is given in Eq. 4.27.

\[
\tilde{\Phi}(q) = \Phi(q) + \Phi_{\text{mod}}(q, \Delta, \ldots)
\]  
\[
\begin{align*}
\Phi(q) & = f(q, \Delta, \ldots) \Phi(q) \\
\Phi_{\text{mod}}(q, \Delta, \ldots) & = f(q, \Delta, \ldots) \Phi_{\text{mod}}(q, \Delta, \ldots)
\end{align*}
\]

In these equations the \( f \) or \( \Phi_{\text{mod}} \) account for the difference between \( \tilde{\Phi}(q) \) and \( \Phi(q) \) due to subgrid scale effects. These quantities can be a function of the flow variables as well as filter width and a number of other parameters. Dynamic models are derived by considering another level of filtering involving a larger scale \( \alpha \Delta \), where \( \alpha > 1 \), and considering the combined filtering at both scales. The second filter (or test filter) is usually denoted by the “hat” symbol, \( \hat{\ldots} \). Using this, one can derive the generalized Germano identity as shown in Eq. 4.28 and 4.29.

\[
\begin{align*}
\Phi(q) + \Phi_{\text{mod}}(q, \alpha \Delta, \ldots) & = \tilde{\Phi}(q) + \Phi_{\text{mod}}(q, \Delta, \ldots) \\
\Phi(q) & = f(q, \alpha \Delta, \ldots) \Phi(q)
\end{align*}
\]

In [70], this approach is used to provide closure for the frame wrinkling factor in the thickened flame model. The flame wrinkling factor was defined here as \( \Xi_{\Delta} = \left| \nabla c \right| / \left| \nabla c \right| \) which allows one to define \( \Phi = |\nabla c| \) and \( f = \Xi_{\Delta} \). A model for \( \Xi_{\Delta} \) is given as shown in Eq. 4.30, but requires closure for the flame
fractal dimension, \( D_f \).

\[
\Xi_{\Delta} = C_f (\delta_\rho/\Delta)^{(2-D_f)} \tag{4.30}
\]

Using the Germano identity an expression can be derived for \( D_f \) by applying the generalized Germano identity as shown in Eq. 4.31.

\[
\Xi_{\Delta} |\nabla \tilde{c}| = \Xi_{a\Delta} |\nabla \tilde{c}| \tag{4.31}
\]

Taking \( C_f \) to be one and substituting Eq. 4.30 into 4.31 for the corresponding filter widths yields Eq. 4.32. Solving for the flame fractal dimension yields the expression in Eq. 4.33 which is a function of filtered progress variable and the filter width, providing closure for a dynamic thickened flame model.

\[
\left( \frac{\delta_\rho}{\alpha \Delta} \right)^{(2-D_f)} \frac{|\nabla \tilde{c}|}{|\nabla \tilde{c}|} = (\delta_\rho/\Delta)^{(2-D_f)} \tag{4.32}
\]

\[
D_f = 2 + \log \frac{|\nabla \tilde{c}|/|\nabla \tilde{c}|}{\log \alpha} \tag{4.33}
\]

Another example of scale-similarity methods in modeling closures looks at decomposing the source term itself. The additive form of the Germano identity is employed by [71] to derive the expressions in Eqns. 4.34 and 4.35.

\[
\bar{\omega}_s(q) = \bar{\omega}_s(\tilde{q}) + \bar{\omega}_{SGS_1} \tag{4.34}
\]

\[
\tilde{\bar{\omega}}_s(q) = \tilde{\bar{\omega}}_s(\tilde{q}) + \tilde{\bar{\omega}}_{SGS_2} \tag{4.35}
\]

The SGS terms can be closed by filtering the above expressions again. This yields Eqns. 4.36 and 4.37.

\[
\bar{\omega}_s(q) = \bar{\omega}_s(\tilde{q}) + \bar{\omega}_{SGS_1} \tag{4.36}
\]

\[
\tilde{\bar{\omega}}_s(q) = \tilde{\bar{\omega}}_s(\tilde{q}) + \tilde{\bar{\omega}}_{SGS_2} \tag{4.37}
\]

Now the first terms in Eqns. 4.36 and 4.37 can be decomposed in the same fashion as Eqns. 4.34 and 4.35.

\[
\bar{\omega}_s(q) = \bar{\omega}_s(\tilde{\tilde{q}}) + \bar{\omega}_{SGS_3} \tag{4.38}
\]

\[
\tilde{\bar{\omega}}_s(q) = \tilde{\bar{\omega}}_s(\tilde{\tilde{q}}) + \tilde{\bar{\omega}}_{SGS_4} \tag{4.39}
\]

Clearly, in Eqns. 4.38 and 4.39, the SGS terms can be equated in terms of the known field and the filtered field. Assuming scale-similarity in the filter levels, the SGS terms in Eqns. 4.34 and 4.35 can be closed as shown in Eqns. 4.40 and 4.41, where \( K_1 \) and \( K_2 \) are scaling constants.

\[
\bar{\omega}_{SGS_1} = K_1 \omega_{SGS_3} = K_1 \left( \frac{\bar{\omega}_s(\tilde{q}) - \tilde{\bar{\omega}}_s(\tilde{q})}{\omega_{SGS_3} - \omega_{SGS_4}} \right) \tag{4.40}
\]
Finally, this yields two scale-similarity closures for the filtered chemical source term as shown in Eqns. 4.42 and 4.43. Eq. 4.42 is the scale-similarity filtered reaction rate model (SSFRRM) and Eq. 4.43 is the scale-similarity resolved reaction rate model (SSRRRM) of [71].

\[
\omega_{SGS} = K_2 \omega_{SGS_i} = K_2 \left( \omega_s(q) - \omega_s(\tilde{q}) \right) 
\]  
(4.41)

\[
\bar{\omega}_s(\rho_s, T) = \bar{\omega}_s(\tilde{\rho}_s, \tilde{T}) + K_1 \left( \bar{\omega}_s(\tilde{\rho}_s, \tilde{T}) - \bar{\omega}_s(\tilde{\rho}_s, \tilde{T}) \right) 
\]  
(4.42)

\[
\bar{\omega}_s(\rho_s, T) = \bar{\omega}_s(\tilde{\rho}_s, \tilde{T}) + K_2 \left( \bar{\omega}_s(\tilde{\rho}_s, \tilde{T}) - \bar{\omega}_s(\tilde{\rho}_s, \tilde{T}) \right) 
\]  
(4.43)

### 4.5 PDF based Methods

The probability density function (PDF) is defined as the derivative of the cumulative distribution function (CDF). The CDF is the probability of any event as defined by Eq. 4.44. Note that \( V \) is the sample space variable corresponding to \( U \). The CDF also has three basic properties; these are described by Eq. 4.45. The third property expresses the fact that the CDF is a non-decreasing function [72].

\[
F(V) \equiv P\{U < V\} 
\]  
(4.44)

\[
F(-\infty) = 0 
\]

\[
F(\infty) = 1 
\]  
(4.45)

\[
F(V_b) \geq F(V_a) \text{ for } V_b > V_a 
\]

The PDF can be defined by Eq. 4.46. It is the derivative of the CDF and satisfies the normalization condition given by Eq. 4.47. More importantly, the PDF can yield the probability of a random variable being in a defined interval by integrating the PDF over the interval, as shown in Eq. 4.48.

\[
f(V) \equiv \frac{dF(V)}{dV} 
\]  
(4.46)

\[
\int_{-\infty}^{\infty} f(V) \, dV = 1 
\]  
(4.47)

\[
P\{V_a \leq U < V_b\} = \int_{V_a}^{V_b} f(V) \, dV 
\]  
(4.48)
Further, the PDF can be used to determine the mean (or expected) values of random variables. The mean of $U$ is defined by Eq. 4.49, which is just the probability weighted average of all values of $U$. Further, the mean of a function of variables can be determined from the function and PDF as shown in Eq. 4.50. [72]

$$
\overline{U} \equiv \int_{-\infty}^{\infty} V f(V) dV 
$$

(4.49)

$$
\overline{Q(U)} = \int_{-\infty}^{\infty} Q(V) f(V) dV 
$$

(4.50)

This is useful for closing the chemical source terms as it is a function of 'random' variables. The filtered chemical source term can be defined based on the PDF of the independent variables as shown in Eq. 4.51. The difficulty now is determining the joint PDF of the species and temperatures.

$$
\overline{\dot{\omega}_s(\rho_s, T)} = 
\int_{Y_1=0}^{1} \int_{Y_2=0}^{1} \cdots \int_{Y_N=0}^{1} \int_{T}^{T} \dot{\omega}_s(Y_1, Y_2, \ldots, Y_N, T) f(Y_1, Y_2, \ldots, Y_N, T) dY_1 dY_2 \ldots dY_N dT 
$$

(4.51)

According to [62], there are two main routes to follow. The first is to presume a shape for the PDF (i.e. using $\beta$-functions or log-normal distributions), determined from the available parameters such as the resolved variables. However, it can be very difficult to assume the shape of a joint pdf dependent on more than two variables. A simplified approach is to assume a statistical independence of the pdf variables to write Eq. 4.52 and assume each of the single variable PDFs. However, this assumption does not hold because all species mass fractions and temperatures are clearly linked in flames.

$$
f(Y_1, Y_2, \ldots, Y_N, T) = f(Y_1) f(Y_2) \ldots f(Y_N) f(T) 
$$

(4.52)

The other route is to derive a balance equation for the filtered pdf. The filtered pdf equation still has a chemical source term, but the sources appear already in closed form. This avoids the problem of modeling an adjustment to the sources based on the mean data. Thus solving the equation for the filtered PDF can yield all of the species mass fractions and temperature using the closed form of the chemical source terms. However, new difficulties arise including the need to close new terms as well as implementation of stochastic models for solving the equation. The exact formulation for the filtered PDF balance equation for a set of reactive scalars varies somewhat in the literature based on assumptions and closure models, but the general form is given in Eq. 4.53 [62, 72]. The terms on the left correspond to unsteady evolution and convection by the mean flow field. The terms on the right correspond to the turbulent convection, molecular mixing, and chemical reaction sources, respectively. The quantity
\(Q(Y = \Psi)\) corresponds to the conditional average of a quantity, \(Q\), for the sampling vector \(\Psi\).

\[
\bar{p} \frac{\partial \tilde{T}}{\partial t} + \bar{p} \bar{u}_j \frac{\partial \tilde{T}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \bar{p}(u''_k Y = \Psi) \right] - \bar{p} \sum_{i=1}^{NS} \sum_{j=1}^{NS} \frac{\partial}{\partial \tilde{\psi}_i} \frac{\partial}{\partial \tilde{\psi}_j} \left[ \tilde{f}D \left( \frac{\partial Y_i}{\partial x_k} \frac{\partial Y_j}{\partial x_k} | Y = \Psi \right) \right] - \bar{p} \sum_{i=1}^{NS} \frac{\partial}{\partial \tilde{\psi}_i} \left( \tilde{f} \tilde{\omega}_i(\Psi) \right)
\] (4.53)

The primary benefit of this method is that the highly non-linear source term is already closed. However, the turbulent advection and molecular mixing terms must be modeled. Pope suggests a gradient diffusion for the turbulent convective flux and a simple mixing model for the diffusion terms [72]. Additionally, this balance equation cannot be solved using conventional discretization schemes. Typically, a Lagrangian scheme is used [73], but Eulerian approaches have been developed as well [74].

In [73], the FDF transport equation is solved using a domain of uniformly distributed particles that evolve in physical and computational space. The evolution in physical space is through the transport equation based on the filtered flow field from the LES solver as given in Eq. 4.54. The particle composition is then updated through mixing and reaction based on 4.55. The particle composition is then used to close the thermodynamic properties to be used in the LES solver. Note that \(x^*\) is the particle position and \(dW\) is the Wiener diffusion term.

\[
dx^* = [\bar{u} + \frac{1}{\bar{p}} \nabla \bar{p}(D + D_T)] \, dt + \sqrt{2(D + D_T)} \, dW
\] (4.54)

\[
d\Psi = -\frac{1}{\tau_{\bar{p}}} (\Psi - \tilde{\phi}) dt + S(\Psi) dt
\] (4.55)

An Eulerian approach is presented by Dodoulas et al. [74] in which the filtered density balance equation is recast as an ensemble of stochastic fields that represent the FDF. A system of stochastic partial differential equations (SPDE’s) for these fields can be derived and is equivalent to the FDF evolution. This SPDE is solved along with the filtered momentum LES equation to provide closure for the velocity field, while the ensemble average of the stochastic fields provide closure for the Favre filtered values of the thermodynamic scalars. The SPDE for the \(k^{th}\) scalar field equivalent in the \(n^{th}\) stochastic field (represented by \(\xi^n_k\)) is given in Eq. 4.56. Again, here we find the sources appearing in the closed form and the Wiener diffusion term. This is the Ito interpretation [75] and features the property that the filtered value of the stochastic term will vanish for a large number of fields. Eq. 4.57 defines that relation of the scalars to the stochastic field. A similar method in which a finite number of moments are evolved to reconstruct the PDF is presented in [76].

\[
\frac{\partial \xi^n_k}{\partial t} + \bar{p} \bar{u}_j \frac{\partial \xi^n_k}{\partial x_j} = \bar{p} \omega_k (\xi^n) - \bar{p} \frac{\tau_m}{\tau_{\bar{p}}} (\xi^n_k - \bar{Y_k}) + \bar{p} \sqrt{2D_e} \frac{\partial \xi^n_k}{\partial x_j} \, dW^n_j
\] (4.56)
\[
\bar{Y}_k = \frac{1}{N} \sum_{n=1}^{N} \xi_k^n
\] 

(4.57)

### 4.6 Reconstruction/Deconvolution Methods

Another method for providing closure for the effects of unresolved turbulence on the chemical source terms involves a reconstruction or deconvolution method in order to recover as much information as possible from the filtered scalar field. If the filtering operator admits an inverse, the complete original field is recoverable. However, LES use filters that are not invertible, and only part of the field can be recovered. In this case, the reconstruction is then called the intermediate scalar. This partially deconvoluted quantity is then used to determine the subgrid-scale part or the total part of the filtered source term, similar to a scale-similarity type model. According to Pantano et al. [77] the deconvolution method is a pure mathematical technique and converges too slowly to the recoverable part of the field. The model developed in [77] involves certain physics that are being resolved in order to decrease the cost of the approximate reconstruction. The intermediate field of a conserved scalar is defined as shown in Eq. 4.58 and is chosen to obtain the subgrid contribution to the filtered value of the chemical sources as shown in Eq. 4.59. The model coefficient, \(c_o\), is defined as a function of the filter size, large scale lengths (\(L_Z\)) and the turbulent Peclet number which is the ratio of turbulent convective transport to diffusive transport [77], \(Pe_t = k^{1/2}L_Z/D\).

\[
Z_M = Z + c_o(Z - \bar{Z}) \\
\dot{\omega}_t = \dot{\omega}_t(Z) + \dot{\omega}_t(Z_M) \quad \text{(4.59)}
\]

\[
c_o = c_o \left( \frac{\Delta t}{2L_Z}, Pe_t \right) \\
\quad \text{(4.60)}
\]

### 4.7 LEM and ODT

Another method that resolves fine grid structures for reactive flow simulations is the one-dimensional turbulence model (ODT). The ODT model was developed as an extension to the Linear Eddy Model (LEM) developed by Kerstein [78]. The stand-alone ODT model is described by Echekki et al [79] as an extension of LEM that maintains a distinction between turbulent stirring and molecular diffusion and reaction. The ODT model is based on the solution of the planar boundary layer equations with constant pressure in the 1D domain. The boundary layer equations for a temporally developing planar flow are given in Eqns. 4.61 - 4.63, where \(t\) and \(y\) are the temporal and spatial coordinates in the 1D domain. Turbulent advection is implemented using stirring events. Several of these 1D domains are used
to simulate a flow while being advected downstream based on the bulk streamwise velocity.

\[
\frac{\partial u}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) \quad (4.61)
\]

\[
\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho} \frac{\partial}{\partial y} \left( \rho Y_k V_k \right) + \dot{\omega}_k / \rho \quad (4.62)
\]

\[
\frac{\partial T}{\partial t} = -\frac{1}{\tau_p} \sum_{k=1}^{NS} c_{p,k} Y_k \frac{\partial T}{\partial y} + \frac{1}{\rho \tau_p} \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) \quad (4.63)
\]

The ODT model can be applied to more complex flows through coupling with LES equations [80, 81]. In this case, an LES grid is used to solve the continuity and momentum equations while ODT elements are overlaid as much finer 1D grids within the LES cells. The temperature and species equations are solved on the ODT elements in order to resolve some of the fine scale effects on the chemical source terms. Species and mixture densities can then be filtered from the ODT domains that make up an LES cell to provide the filtered scalar fields.

A problem with closure models such as ODT, FDF or even the PaSR models is that they incur additional complexity and cost to the already expensive LES calculations necessary to resolve the types of flows being considered. ODT cost increases with the refinement of the 1D domain, while the FDF models require seeding of a large number of particles as well as additional equations to be solved. The extended PaSR model of Fureby et al. [69] requires the solution of additional species equations and an energy equation for the fine-scale structures. Adding this cost to the already expensive computational requirements to resolve supersonic internal flows (such as the 60 M cell mesh required for configuration E in this work) is not negligible. Further, these methods add additional complexity. The ODT methods require a complex method of solving and coupling the 3D LES equations with the refined 1D domains, which also must be oriented to traverse the large gradients of the flow. The FDF models are even more complicated since they take a completely different approach for describing the flow and require the tracking of a large number of stochastic particles. Even in the case of the Eulerian versions [74], multiple sets of equations need to be solved in order to get an estimate of the FDF.

4.8 Previous Models by NCSU’s Hypersonics Group

The hypersonics CFD lab at NCSU has done previous work in developing closure models for chemical source terms in turbulent reacting flow as well. Potturi and Edwards present several models that draw from PaSR and scale-similarity ideas in [48]. The intent in deriving these models has been to develop techniques that allow for sub-cell effects and finite-rate chemistry but do not incur excessive computational complexity. Simulations incorporating these models were compared to those using lami-
nar chemistry as well as experimental data in the dissertations of Potturi [40] and Fulton [2] for different scramjet configurations.

### 4.8.1 PaSR(0) Closure

The models presented in [48] include PaSR type models as well as scale-similarity models. The first model is the PaSR(0) closure which model the filtered species source terms as shown.

\[
\overline{\omega}_s \approx \frac{\rho \overline{\omega}_s(\overline{\rho}_s, \overline{T})}{\overline{\rho} + c_1 t_{SGS} \max\left(||\overline{\omega}^+||, ||\overline{\omega}^-||\right)} \tag{4.64}
\]

In this model, \(c_1\) is a constant and \(t_{SGS}\) is the characteristic time scale of the subgrid fluctuations as given by Eq. 4.65.

\[
t_{SGS} = \max\left(\frac{\Delta}{\gamma^2, u_{SGS}}\right) \tag{4.65}
\]

\[
u_{SGS} = \sqrt{\frac{2}{3} \sum_k \left[\overline{u_k^2} - \overline{\overline{u_k}}^2\right]} \tag{4.66}
\]

A feature of this model is that it only allows for attenuation of reactivity, that is, the model source term will always be less than or equal to the source based on the resolved data. The constant \(c_1\) is determined based on *apriori* analysis of fine grid data. Note that this model incorporates the ‘positive’ and ‘negative’ parts of the chemical sources separately (see Section 2.3).

### 4.8.2 PaSR(1) Closure

The next model presented is the PaSR(1) closure, which is derived assuming that each computational cell consists of fine-scale and coarse structures. In this case, the average filtered chemical source term is defined as shown in Eq. 4.67, where \(^*\) denotes the fine-scale structures, \(^o\) denotes the coarse structures, and \(\gamma^*\) is the volume fraction of the fine-scale structures.

\[
\overline{\omega}_s = \gamma^* \overline{\omega}_s(\rho^*_s, T^*) + (1 - \gamma^*) \overline{\omega}_s(\rho^o_s, T^o) \tag{4.67}
\]

In [48] the governing equations for the fine-scale structures were derived in terms of the fine-scale and LES resolved variables. The governing equation for fine-scale species density and mixture enthalpy are given in Eqns. 4.68 and 4.69, respectively. These equations require definitions for the volume fraction of the fine-scale structures \(\gamma^*\) and the characteristic time scale of mass and energy exchange between
the fine and coarse structures, $t_m$.

\[
(1 - \gamma^*)(\frac{\partial \rho^*_s}{\partial t} + \frac{1}{\kappa} \int_A \rho^*_s \gamma^* u_j \cdot n_j dA) - \frac{1}{t_m} (\bar{\rho}_s - \rho^*_s) = (1 - \gamma^*) \omega_s (\rho^*_s, T^*)
\] (4.68)

\[
(1 - \gamma^*) \left( \frac{\partial}{\partial t} \left( \sum_{s=1}^{NS} \rho^*_s h_s(T^*) \right) + \frac{1}{\kappa} \int_A \sum_{s=1}^{NS} \rho^*_s h_s(T^*) \gamma^* u_j \cdot n_j dA \right)
\]

\[- \frac{1}{Pr} t_m \bar{c}_{p,\text{mix}} (\bar{T} - T^*) - \frac{1}{t_m} \sum_{s=1}^{NS} h_s (\bar{T} (\bar{\rho}_s - \rho^*_s) = 0
\] (4.69)

Several closures were proposed for defining $\gamma^*$ and $t_m$. Eqns. 4.70 and 4.71 are definitions provided by Giacomazzi et al. [82] where $l_k = \Delta \pi^{-1/6} Re^{-1/2}$ and $Re_\Delta = \frac{\bar{u}_{sgs} \Delta}{\bar{B}}$. The assumption in the PaSR models of Giacomazzi et al. is that the reactions primarily occur in the fine-scale structures. This differs from the PaSR(1) model which makes no such assumption, and takes into consideration the reactions occurring in both the fine and coarse-scale structures.

\[
t_m = Sc l_k^2 \bar{B}
\] (4.70)

\[
\gamma^* = \left( \pi^{-1/6} Re_\Delta^{-1/2} \right) \log(\pi) \log(\pi^{1/6} Re^{1/2})
\] (4.71)

Also used is the model for the mixing time and volume fraction provided by Fureby et al. as shown in Eqns. 4.72 and 4.73, which makes similar assumptions to that of the PaSR(1) model [68, 69].

\[
t_m = \frac{\Delta}{u_{sgs}} Re_\Delta^{-1/4}
\] (4.72)

\[
\gamma^* = \frac{t_c}{t_c + t_m}
\] (4.73)

The models from the eddy dissipation concept (EDC) are also presented in Eqns. 4.74 and 4.75 as a final option for completing the model [83].

\[
t_m = 0.9075 \frac{\Delta}{u_{sgs}} Re_\Delta^{-1/2}
\] (4.74)

\[
\gamma^* = 0.876 Re_\Delta^{-3/4}
\] (4.75)

The PaSR(1) model involves using one of the three closure methods for the time scale and fine-scale structure volume fraction to close Eqns. 4.68 and 4.69. These equations are solved in addition to the main LES flow equations. The difference between this model and others from the literature is the
inclusion of convective transport of fine-scale structures (similar to [69]) and the alternative expressions for the subgrid mixing time and volume fraction of fine-scales. A comparison of this model to other PaSR models can be found in [48].

4.8.3 PaSR(2) closure

A modified form of PaSR(0) was defined and implemented in [2]. The modified form is given below, where \( t_c \) is defined as shown in Eq. 4.77. Note that the ‘positive’ and ‘negative’ components in Eq. 4.77 are evaluated using laminar chemistry.

\[
\bar{\omega}_s \approx \frac{t_c \bar{\omega}_s(\bar{\rho}_s, \bar{T})}{\max\left(t_c, \frac{\text{Re}_\Delta - 1}{\text{Re}_\Delta} t_{SGS}\right)} \tag{4.76}
\]

\[
t_c = \frac{\bar{\rho}}{\max\left(||\bar{\omega}^+||, ||\bar{\omega}^-||\right)} \tag{4.77}
\]

\[
\text{Re}_\Delta = \frac{\max(u', \nu/\Delta) \Delta}{\nu} \tag{4.78}
\]

The definition of \( t_{SGS} \) is the same as for the PaSR(0) model (Eq. 4.65), and \( \Delta \) is the mesh width. This model is designed to force the scaling factor to 1 as \( \text{Re}_\Delta \to 1 \) so that laminar chemistry assumption is recovered when there is no turbulence.

4.8.4 PaSR/Scale Similarity Model (PaSR-SS)

Another model presented in past work is the PaSR(SS) model in which the time scale ratio used in the PaSR(0) is defined based on information from the source terms determined by test-filtered data. The intent here is to determine an estimate for the ‘un-mixedness’ of the solution for a corresponding cell based on the test-filtered data. The model is defined by Eq. 4.79.

\[
\bar{\omega}_s = \min\left(c_3, c_1 \frac{||\bar{\omega}_s(\bar{\rho}_s, \bar{T})|| + c_2 \mu / \Delta^2}{||\bar{\omega}_s(\bar{\rho}, \bar{T})|| + c_2 \mu / \Delta^2}\right) \bar{\omega}_s(\bar{\rho}_s, \bar{T}) \tag{4.79}
\]

This model allows for both attenuation and augmentation of chemical sources requiring additional constants \( c_3 \) and \( c_2 \). \( c_3 \) is the maximum allowed enhancement of reactivity and is usually set to 2-3. Numerical difficulties are avoided by adding a small factor to both the numerator and denominator with \( c_2 = 0.1 \). Again, \( c_1 \) is determined based on a priori analysis, presented in [48].
4.8.5 Scale Similarity Model (SS)

The final model considered in NCSU’s prior work is the pure scale-similarity model (SS). This model is directly motivated by the model of simple SGS terms [71]. The model is given in Eq. 4.80 and was tested for dual-mode ramjet/scramjet combustor simulation along with the other models.

\[
\bar{\omega}_s = \omega_s(\bar{\rho}_s, \bar{T}) + c_1 \left[ \omega_s(\bar{\rho}_s, \bar{T}) - \omega_s(\bar{\rho}_s, \bar{T}) \right]
\]

(4.80)

Due to the nature of the non-linear chemical sources, it is highly probable that this model will attenuate reactivity rather than enhance. This is because filtering the resolved data results in ‘artificial mixing’ of reactants and heat. If this filtering occurs in a region of cells that, separately, are not reactive but together result in a reactive mixture, this will result in very large source terms. This can also take place if filtering occurs in a location where a hot mixture of products is filtered with a region of colder reactants that have not been heated to the activation energy.

4.8.6 Summary of Results

The previous models developed by our group were developed based on a traditional *a priori* analysis. This analysis was performed using data extracted from a reactive flow simulation of the UVa combustor corresponding to configuration A (see Section 5.2.1). Filtered data from the fine-mesh LES was used to evaluate the PaSR(0), PaSR(SS), and SS models in order to determine optimal constants. This analysis involved comparing two different ‘merit’ functions. One is the \(L^2\) norm of the species production rates; the other is a measure of temperature change per unit time. Comparisons were made between the modeled merit function on the coarse grid (which was filtered from the fine grid solution) to the filtered fine-mesh merit function. The correlation and slope are determined for a range of model constants for each model; these two quantities are compared for each model along with laminar chemistry. The optimal model constants are those that result in correlation and slopes of unity. This analysis is discussed in detail in [48].

The relative expensive of each model should also be noted. The PaSR(1) model is the most expensive as it requires the addition of one plus the number of species equations to the system of equations being solved. The PaSR(SS) and SS models also add to the cost of the simulation due to the requirement of filtering and re-evaluating the chemical source terms. This becomes increasingly expensive as the numbers of species and reactions increase. The cheapest are the PaSR(0) and PaSR(2) models which require no filtering or additional chemical production rate calculations.

The models were tested on three cases. In [40, 48] the models are compared against experimental data for the German Aerospace Center’s (DLR) combustor as well as experimental configurations at the University of Virginia (UVa). For the case of the DLR combustor [84, 85], axial velocity profiles,
temperature profiles, and axial velocity fluctuation profiles are available for comparison. For the UVa configurations, results were compared against experimental CARS measurements. In [2], two models were compared against laminar chemistry results as well as experimental data for a hydrogen fueled scramjet combustor.

In [40, 48] it was found that all subgrid models predict very similar results for the DLR combustor. More pronounced differences were observed in comparing results for one of the hydrogen fueled cases. The PaSR(0) model resulted in the lowest temperatures. Best visual comparisons with the CARS data was achieved when using the PaSR(SS) model. The subgrid closure models used resulted in decreased magnitude of species production compared to laminar chemistry; the most aggressive was the PaSR(0) model. A performance metric was also defined in [40, 48] to measure the improvement due to each model for the scramjet combustor. This was done by comparing the error of simulation results relative to the experiment. This analysis revealed that the scale-similarity model resulted in the most improvement, but this was only a “modest” improvement.

In [2] the PaSR(0) and PaSR(2) models were implemented for a scramjet combustor with a ramp injector. The results for the PaSR(0) model predicted a detachment of the flame from the compression ramp resulting in a lifted flame. The PaSR(2) model matched more closely with the experiment with no flame detachment. However, downstream of ignition, the mean temperatures were very similar to that predicted by laminar chemistry. The models also improved temperature fluctuation agreement with the experiment.

The conclusion from these studies was that, although the models appear promising from a priori analysis, they do not perform as well in a posteriori testing. This is partially due to the nature of the classical a priori analysis which builds models based on the idea that a filtered set of data can be used to evaluate chemical source terms representative of an evolved course grid solution. In general, the filtered chemical production rates are much smaller than the production rates evaluated using filtered flow data. This leads to models that are calibrated to over-attenuate reactivity, which explains the results found in [2] when using the PaSR(0) model. These findings lead to the motivation of a mesh-sequenced approach for the assessment of these types of combustion closure models. In this case, the finest mesh in a sequence of grids would be considered the ‘truth model’, and would provide a local, instantaneous target for subgrid-scale model development. This is discussed in the following section.
4.9 Towards a New Family of Models

4.9.1 Mesh-Sequenced Realizations

In developing a new family of turbulent closure models for high-speed combustion, simultaneous mesh-sequenced realizations are used. Mesh-sequenced realizations are utilized to study the effect of unresolved turbulence on the coarse-mesh chemical production rates relative to those from the fine grid LES. By comparing the chemical production rates evaluated using laminar chemistry between fine- and coarse-mesh simulations, the error in the chemical source terms associated with the unresolved turbulence on the coarse-mesh can be quantified.

Several modifications to the REACTMB code were required to enable simultaneous mesh-sequenced large-eddy simulations to be performed. REACTMB already has logic to handle multi-block, structured grids, and connectivity files are used to set boundary conditions and connect blocks. To set up a hierarchy of parent to children information-passing, some considerations have to be made. In this case, the fine grid blocks are considered the parent, which pass information to the children: the coarse grid blocks corresponding to that of the parent blocks. For simplicity, the parent and children blocks are assigned to the same processors to avoid having to pass information among all nodes. Further, the parent blocks must be evolved first in every iteration followed by the children. This requires assigning an order to the local blocks on each processor. Routines are added to pass information such as chemical production rates or velocity field data from the underlying fine grid to the coarser grids. Finally, logic must be in place to filter the fine-mesh data appropriately to the coarse-grid resolution. For example, Eqn. 4.81 defines the volume weighted filtering approach from a fine resolution to a grid level with twice the mesh width. Here, $\bar{q}_f$ is the generic flow variable filtered from the fine-grid, $\tilde{q}_f$ is the generic flow variable resolved by the fine-grid, and $V_{CV}$ is the cell volume. The summation takes place over eight cells since one level of refinement in 3D space results in eight fine-grid cells for every coarse-grid cell.

$$\bar{q}_f = \frac{\sum_{k=1}^{8} V_{CV,k} \tilde{q}_{f,k}}{\sum_{k=1}^{8} V_{CV,k}}$$  (4.81)

An important part of this analysis relies on a method for coupling the velocity field. This is essential to correlate the eddy structures between the fine grid with those on the coarse grids. Several methods for coupling the velocity fields were employed including a direct filtering approach. This involved filtering the fine-grid velocity information using Eq. 4.81 and directly substituting it for the coarse-grid velocity field. However, the best method, one that resulted in instantaneous eddy structures that were similar among grid levels as well as minimal error in time averaged statistics, involved adding a momentum source term that ‘relaxed’ the fine-grid velocity information onto the coarser grid level. The LES momentum equation (Eq. 2.60) can be modified to include this source term as shown below, where $\bar{u}_{i,f}$ is
the velocity field filtered from the fine grid solution, using a filtering method such as in Eq. 4.81. The time scale $1/\tau$ is given by Eq. 4.83, where $U_c = 0.8\sqrt{u'^2 + v'^2 + w'^2}$ is an estimate of the convective eddy velocity.

$$\frac{\partial \rho \overline{u_i}}{\partial t} + \frac{\partial \rho \overline{u_i u_j}}{\partial x_j} + \frac{\partial \rho}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = \frac{1}{\tau} \rho \left( \overline{u_i f} - \overline{u_i} \right)$$

(4.82)

$$\frac{1}{\tau} = \frac{U_c}{\lambda_l}$$

(4.83)

Also required is an estimate of the integral length scale. This is defined by Eq. 4.84, where the length scale is expressed as a multiple of the turbulent mixing length calculated from the time-averaged modeled turbulent kinetic energy, time-averaged turbulence frequency, and the resolved turbulent kinetic energy. Here $C_I = 5, C_\mu = 0.09$, and $\kappa$ is the von Kármán constant.

$$\lambda_l \equiv C_I l_{mix}$$

$$l_{mix} = \min \left( \kappa d, 1.5 \sqrt{\frac{10\nu \overline{\omega} + \overline{k} + k_R}{C_{1/2} \overline{\omega \overline{\omega}}}} \right)$$

(4.84)

$$k_R = \frac{1}{2\rho} \left( \rho \overline{u_i u_k} - \frac{\rho \overline{u_k} \rho \overline{u_k}}{\rho} \right)$$

Results from testing this coupling method for a pure mixing case is discussed in Section 5.1.1.

Earlier studies in this work involved the evolution of three different grid levels in this mesh-sequenced framework. The finest grid level was taken to be the ‘truth model’ which passed information to the lower grid levels. The general trend observed for the reactive test case, is that temperatures, flame thickness, and volumetric expansion of the flame all increase as the grid is coarsened. Also, there was no clear correlation between eddies, as the fine grid would resolve finer scales resulting in a different evolution of the turbulent structures. Using the capabilities described above, it was found that by coupling the velocity fields between the coarser grids and the fine grid, instantaneous eddy evolution was very similar between grid levels. The coarser grid levels resulted in ‘smeared’ versions of the fine-mesh structures. Due to this coupled field, however, the volumetric expansion enabled on the coarser grids was constrained and the flame temperatures further increased. Fortunately, this is corrected when filtered fine-mesh chemical production rates are imposed on the coarser grid levels. This leads to the conclusion that the filtered-fine grid chemical source terms, evaluated using laminar chemistry, should serve as the target for a combustion closure model on the coarse grids.

### 4.9.2 Modified a priori Analysis

Given the capabilities and observations described in the previous section, filtered fine grid chemical source terms can be used as a model target for subgrid-scale closure models. However, in practice,
fine-mesh information will not always be available. This means that closure is still required to define a model to account for turbulent fluctuations. The approach taken in this work was a modified a priori approach, in which fine- and coarse-mesh simulations are evolved separately. The reason for the use of this approach is that the traditional approach of filtering fine-mesh data and evaluating chemical source terms to represent a coarse-mesh field overestimates the coarse grid chemistry. However, a complexity arises since the fine- and coarse-mesh simulations will develop different eddy structures that are not comparable. To address this, velocity coupling must again be used so that the eddy structures are highly correlated. This allows a direct comparison of chemical source terms at discrete points and space and time between two grid levels.

In order to make comparisons, data at discrete locations must be extracted over a number of time steps. The data extracted should include relevant quantities such as species densities, temperature, pressure, flow velocity and any other variable required to evaluate desired parameters. Considerations must be made in order to test any filtering operations as well; data from a number of neighboring cells is required to test these effects. Further, fine grid information must be extracted as well, in order to compare with the corresponding coarse grid information.

Using a large database of extracted information, the postulated closures can be analyzed to see if they resulted in corrections to the coarse-grid chemical source terms that match with the filtered fine-grid values. The dataset can also be used to seek correlations between the fine grid sources and other quantifiable variables such as mixture fraction or Damköhler number. In this work, several closed forms have arisen from this analysis including models based on test-filtered chemical source terms, scale-similarity arguments, and correlations for predicting an ‘optimal single point’ in the neighborhood of coarse grid cells that is representative of the fine grid chemical sources. Given proposed closures, the dataset can then be used to compare adjusted reactivity measures (such as individual chemical production rates or heat release) to assess the models. It should also be noted that this data set also includes information analogous to a traditional a priori analysis; the fine-mesh flow data can be filtered down to the coarse grid resolution to provide another coarse grid ‘realization’ for comparison. Results and discussion from the modified a priori analysis can be found in Section 5.1.2. The following section describes a new class of subgrid-scale models that were developed based on this mesh-sequenced realization / modified a priori approach.

4.10 A New Family of Models

The subject of this dissertation is in the derivation, assessment, and application of a new family of turbulence combustion closure models based on mesh-sequenced realizations of a turbulent reacting flame. The model is derived based on a least-squares minimization between the fine grid and coarse grid chemical source terms. Matching the resolved source terms of the fine grid is desired based on the
observations from the mesh-sequenced realizations described in Section 4.9.1.

### 4.10.1 Derivation of the General Form

The general form of our new model is defined below.

\[
\dot{\omega}_s(q) = f(\tilde{q}, \Delta, \ldots) \dot{\omega}_s(\tilde{q})
\] (4.85)

The enhancement factor, \( f \), is designed to account for the unresolved turbulent fluctuations as a function of the resolved flow variables as well as other quantities such as grid scale or local Damköhler number.

In practice, \( \dot{\omega}_s \) is the modeled sources, but in seeking correlations for determining appropriate models of \( f \), we used mesh sequenced realizations to compare the filtered fine grid sources and the coarse grid sources. If we define the modeled source as the filtered fine grid source, \( \dot{\omega}_sf \), we can derive an expression for the enhancement factor that minimizes the difference between the modeled sources and the fine grid sources. This is done by taking the \( L^2 \) norm of the difference between the two as shown in Eq. 4.86.

\[
g(f) = ||\dot{\omega}_sf - f\dot{\omega}_s||^2 = \sum_{s=1}^{NS} (\dot{\omega}_sf - f\dot{\omega}_s)^2
\] (4.86)

Minimizing this equations requires taking the derivative of the function, \( g(f) \), and setting it to zero.

\[
\frac{dg}{df} = \sum_{s=1}^{NS} (\dot{\omega}_sf\dot{\omega}_s - f\dot{\omega}_s\dot{\omega}_s) = \sum_{s=1}^{NS} \dot{\omega}_sf\dot{\omega}_s - f \sum_{s=1}^{NS} \dot{\omega}_s\dot{\omega}_s = 0
\] (4.87)

This yields the ‘exact’ least-squares minimization (LSM) model as shown in Eq. 4.88.

\[
f_{\text{exact}} = \frac{\sum_{s=1}^{NS} \dot{\omega}_sf\dot{\omega}_s}{\sum_{s=1}^{NS} \dot{\omega}_s\dot{\omega}_s}
\] (4.88)

From here, a closure model can be derived in a variety of ways. The general closure is defined by Eq. 4.89, where the different model formulations will provide expressions for \( \dot{\omega}_s \) and \( \dot{\omega}_f \). The second term in both the numerator and denominator is added to ensure that division by zero does not occur. This limiting term is defined to be dimensionally consistent with the other terms; it can be derived by multiplying the smallest turbulent time scale resolvable on a mesh \( (\nu/\Delta^2) \) by the local density.

\[
f = \min \left[ A, \frac{\sum_{s=1}^{NS} \dot{\omega}_s\dot{\omega}_s + (B\frac{\mu}{\Delta})^2}{\sum_{s=1}^{NS} \dot{\omega}_s\dot{\omega}_s + (B\frac{\mu}{\Delta})^2} \right]
\] (4.89)

The constant \( B \) is a small number that is set to 0.1 in this work. The \( A \) constant is the maximum allowable value of the enhancement factor. By setting the constant \( A = 1 \) only attenuation is allowed. Usually \( A \) is
set to 3 to allow for some level of enhancement, unless otherwise noted. A limiting factor of 3 is chosen based on PDFs which indicate that the ratios of chemical production rates between fine- and coarse-mesh levels range between -3 and 3 (see Figure 5.18). Further extensions can be made by seeking correlations between flow quantities and the exact formulation to adjust the baseline model.

It should be noted that this model scales all chemical production rates by a single constant. The primary advantage of doing so is that conservation of mass is still maintained without any other considerations. Although not consistent with the least-squares minimization framework, it is possible that defining different enhancement factors for each species would provide additional improvement. However, the issue of mass conservation would need to be addressed. Some multi-variable optimization procedure could potentially be used to derive a model similar to LSM for determining individual enhancement factors for each species. Splitting of the chemical production rates into positive and negative parts, and scaling these components, is another alternative that could provide additional benefit.

### 4.10.2 Filtered Source Closure (LSM-FS)

The first closed model form is the LSM-FS model. This model replaces the filtered fine grid sources with filtered source terms that are resolved at a given grid resolution. The LSM-FS model is defined by combining Eqns. 4.90 and 4.89. The models are formulated using the absolute value signs to ensure that the sign of the enhancement factor is positive. This prevents the flipping of signs of all of the chemical production rates, which would result in the simulation becoming unstable.

\[
\bar{\omega}_s = \hat{\omega}_s(\tilde{q})
\]

\[
\bar{\omega}_s = \text{sign}(\hat{\omega}_s) |\hat{\omega}_s(\tilde{q})|
\]  

(4.90)

The general test filter is defined as shown in Eq. 4.91 for general filter weights \((\alpha_k)\) in the neighborhood of 27 cells surrounding a given cell.

\[
\hat{\omega}_s = \alpha \sum_{k=1}^{27} \alpha_k \hat{\omega}_{s,k}
\]  

(4.91)

The weights \((\alpha_k)\) in the filtering option can be varied to obtain filter widths of \(\Delta\) or \(2\Delta\) as defined by Table 4.1. In this study, a filter width of \(2\Delta\) is normally used, unless otherwise noted. This model allows for both attenuation and enhancement of reactivity.

### 4.10.3 Minmod Extension (LSM-MMD)

An extension of the LSM-FS model is the LSM-MMD model, where MMD denotes the use of a minmod operation. This model ensures that only attenuation is allowed by defining the filtered source term as the minimum between the filtered and resolved source terms for a given cell. The model closures are
Table 4.1: $\alpha$ coefficients for test filter widths of $\Delta$ and $2\Delta$.

<table>
<thead>
<tr>
<th>$k$</th>
<th>i-index</th>
<th>j-index</th>
<th>k-index</th>
<th>$\alpha_k(2\Delta)$</th>
<th>$\alpha_k(\Delta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>i</td>
<td>j</td>
<td>k</td>
<td>1/8</td>
<td>27/64</td>
</tr>
<tr>
<td>2</td>
<td>i-1</td>
<td>j</td>
<td>k</td>
<td>1/16</td>
<td>9/128</td>
</tr>
<tr>
<td>3</td>
<td>i+1</td>
<td>j</td>
<td>k</td>
<td>1/16</td>
<td>9/128</td>
</tr>
<tr>
<td>4</td>
<td>i</td>
<td>j-1</td>
<td>k</td>
<td>1/16</td>
<td>9/128</td>
</tr>
<tr>
<td>5</td>
<td>i</td>
<td>j+1</td>
<td>k</td>
<td>1/16</td>
<td>9/128</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>j</td>
<td>k-1</td>
<td>1/16</td>
<td>9/128</td>
</tr>
<tr>
<td>7</td>
<td>i</td>
<td>j</td>
<td>k+1</td>
<td>1/16</td>
<td>9/128</td>
</tr>
<tr>
<td>8</td>
<td>i-1</td>
<td>j-1</td>
<td>k</td>
<td>1/32</td>
<td>3/256</td>
</tr>
<tr>
<td>9</td>
<td>i+1</td>
<td>j-1</td>
<td>k</td>
<td>1/32</td>
<td>3/256</td>
</tr>
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<td>j+1</td>
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</tr>
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<td>1/32</td>
<td>3/256</td>
</tr>
<tr>
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<td>k+1</td>
<td>1/32</td>
<td>3/256</td>
</tr>
<tr>
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</tr>
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<td>j</td>
<td>k-1</td>
<td>1/32</td>
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</tr>
<tr>
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<td>i</td>
<td>j-1</td>
<td>k-1</td>
<td>1/32</td>
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</tr>
<tr>
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<td>1/512</td>
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<td>23</td>
<td>i+1</td>
<td>j-1</td>
<td>k+1</td>
<td>1/64</td>
<td>1/512</td>
</tr>
<tr>
<td>24</td>
<td>i-1</td>
<td>j-1</td>
<td>k-1</td>
<td>1/64</td>
<td>1/512</td>
</tr>
<tr>
<td>25</td>
<td>i-1</td>
<td>j+1</td>
<td>k-1</td>
<td>1/64</td>
<td>1/512</td>
</tr>
<tr>
<td>26</td>
<td>i+1</td>
<td>j+1</td>
<td>k-1</td>
<td>1/64</td>
<td>1/512</td>
</tr>
<tr>
<td>27</td>
<td>i+1</td>
<td>j-1</td>
<td>k-1</td>
<td>1/64</td>
<td>1/512</td>
</tr>
</tbody>
</table>

summarized by Eq. 4.92.

$$\omega_s = \hat{\omega}_s(\bar{\theta})$$

$$\overline{\omega}_s = \text{sign}(\hat{\omega}_s) \min \left[ |\hat{\omega}_s(\bar{\theta})|, |\hat{\omega}_s| \right] \quad (4.92)$$

This model does not allow for enhancement of reactivity and should be further biased to increased attenuation compared to the LSM-FS model as it will always take the minimum source values. It should be noted that this is not the same as clipping the LSM-FS model at a value of one, since this acts on each individual species production rate, not the enhancement factor itself.
4.10.4 Scale-Similarity Closure (LSM-SS)

Another option is a true scale-similarity type model that involves evaluating the chemical source terms based on test filtered field variables. This is referred to as the LSM-SS model in this work. The LSM-SS model is summarized in Eq. 4.93.

\[
\dot{\omega}_k = \dot{\omega}_k(\hat{\varphi}) \\
\bar{\omega}_k = \text{sign}(\dot{\omega}_k) \left| \dot{\omega}_k(\hat{\varphi}) \right|
\]  

(4.93)

This model allows for both attenuation and augmentation of reactivity in its standard form. However, since filtering the field variables tends to result in ‘artificial mixing’ of both reactants as well as temperature, the source terms evaluated using the filtered variables are generally much larger than the resolved sources. This means that this model should generally be much more attenuative than the other models. Further, this model is the most expensive in the new family of models in that it requires filtering of the source terms and flow variables as well as a second evaluation of the chemical production rates.

4.10.5 Inclusion of Heat Release (LSM-H)

To build on the models, a dependence on heat release can be added. This involves adding to the numerator and denominator a product of heat release in an analogous fashion to the source terms. The general model with heat release can be expressed as shown in Eq. 4.94, where \( C \) is a scaling constant based on an estimation of mixture enthalpy.

\[
f_H = \min \left[ A \frac{\sum_{s=1}^{NS} \bar{\omega}_s \dot{\omega}_s + C^2 \left( \sum_{s=1}^{NS} h_{f,s}^0 \bar{\omega}_s \right) \left( \sum_{s=1}^{NS} h_{f,s}^0 \dot{\omega}_s \right) + \left( B \frac{H}{S^2} \right)^2}{\sum_{s=1}^{NS} \dot{\omega}_s \bar{\omega}_s + C^2 \left( \sum_{s=1}^{NS} h_{f,s}^0 \dot{\omega}_s \right) \left( \sum_{s=1}^{NS} h_{f,s}^0 \bar{\omega}_s \right) + \left( B \frac{H}{S^2} \right)^2} \right]
\]

(4.94)

\[
C = \frac{1}{c_{p,\text{mix}} T}
\]

(4.95)

\[
c_{p,\text{mix}} = \sum_{s=1}^{NS} Y_s c_{p,s}(T)
\]

(4.96)

The notation can be simplified by defining the heat release terms as shown below.

\[
q_H = \sum_{s=1}^{NS} h_{f,s}^0 \dot{\omega}_s
\]

\[
\bar{q}_H = \text{sign}(q_H) \left| \sum_{s=1}^{NS} h_{f,s}^0 \bar{\omega}_s \right|
\]

(4.97)
Now the general model with heat release can be rewritten as shown in Eq. 4.98.

\[
f_H = \min \left[ A, \sum_{s=1}^{NS} \bar{\omega}_s \bar{\omega}_s + C^2 qH qH + \left( B \frac{\mu}{\overline{\nu}} \right)^2 \right]
\]

(4.98)

Now we can define another family of models with heat release. For example an exact LSM with heat model can be defined by combining 4.97, 4.98, and 4.99.

\[
\dot{\omega}_s = \dot{\omega}_s(\bar{q})
\]

\[
\bar{\omega} = \bar{\omega}_s(\bar{q}) = \bar{\omega}_sf
\]

(4.99)

Further, we can define models based on the filtered sources alone with heat release by combining Eqns. 4.90, 4.97, and 4.98 to define the LSM-FS-H model. A scale-similarity with heat model can be defined by combining equations 4.93, 4.97, and 4.98 to give the LSM-SS-H model.

### 4.10.6 Single Point Correlations

Through the modified *a priori* analysis incorporated in this study (see section 4.9.2), it was discovered that there exists a single cell in the neighborhood of 27 cells that could be defined as the modeled filter sources in Eq. 4.89 that greatly reduces scatter when comparing model numerators. This was an exciting development because it implies that the information to model the fine filtered source terms existed in the field of the resolved space; however, correlating variables to correctly choose this cell has proven to be difficult. It was also found that only considering a subset of the species resulted in only a slight increase in scatter. This means that only one or two of the major species (fuel, oxidizer, or water) needs to be considered. Given exact fine grid data, the exact single point model can be defined by Eqn. 4.100.

\[
\dot{\omega}_s = \dot{\omega}_s(\bar{q})
\]

\[
\bar{\omega}_s = \bar{\omega}_s|_{k=M}
\]

\[
\bar{\omega}_s|_{k=M} = \arg \min \left[ |\bar{\omega}_{H_2O f} - \bar{\omega}_{H_2O,k}| \right]
\]

(4.100)

Here, cell \( M \) is the cell that minimizes the absolute value of the difference between the fine filtered and resolved chemical source terms for water. The source vector of the cell that minimizes the difference, in the neighborhood of 27 cells, is taken to be the model filtered source vector.

In order to develop a model that doesn’t require fine grid data, artificial neural networks in the JMP-Pro program were used to model a function for the difference between the fine filtered and local resolved water source terms. This function, \( Z \), was trained on a set of tabulated data of temperature, resolved water source term and the species mass fraction of hydrogen, oxygen, and water from the 3D
hydrogen-air reacting shear layer discussed in chapter 5. The function is meant to predict the difference between the fine filtered water source term corresponding to a cell $i$ and the resolved water source term of cell $k$ surrounding cell $i$. The single point model using the JMP-ANN fit is defined by Eq. 4.101.

$$
\dot{\omega}_s = \dot{\omega}_s(q) \\
\overline{\dot{\omega}_s} = \dot{\omega}_s|_{k=n} \\
\dot{\omega}_s|_{k=n} = \arg \min \left[ |Z(\dot{\omega}_{H_2O}, Y_{H_2}, Y_{O_2}, Y_{H_2O}, T)_k| \right] \tag{4.101}
$$

Another method for predicting the ‘optimal single point’ in the neighborhood of 27 cells was to define a reduced reactivity measure for each of these cells as defined in Eq. 4.102, where $||\dot{\omega}||_{\text{max}}$ and $||\dot{\omega}||_{\text{min}}$ are the local maximum and minimum $L^2$ norms of the chemical production rates, respectively.

$$
R_k = \frac{||\dot{\omega}||_k - ||\dot{\omega}||_{\text{min}}}{||\dot{\omega}||_{\text{max}} - ||\dot{\omega}||_{\text{min}}} \tag{4.102}
$$

Using this reduced reactivity measure results in a local quantity, varying between zero and one, that indicates a relative reactivity measure of every cell in the neighborhood. Given the fine grid data, the value $R_M$ can be defined for the optimal single point cell as defined by Eq. 4.100. Seeking correlations to predict $R_M$ based on coarse grid data only is now the task. Correlations for the most probable $R_M$ value based on Damköhler number and mixture fraction are discussed in Section 5.1.2. Given a model for predicting $R_M$, the LSM-$R_M$ model can be evaluated using Eq. 4.103.

$$
\dot{\omega}_s = \dot{\omega}_s(q) \\
||\dot{\omega}||_t = R_M(||\dot{\omega}||_{\text{max}} - ||\dot{\omega}||_{\text{min}}) + ||\dot{\omega}||_{\text{min}} \\
\dot{\omega}_s|_{k=n} = \arg \min \left[ \text{abs}(||\dot{\omega}||_t - ||\dot{\omega}||_k) \right] \\
\overline{\dot{\omega}_s} = \dot{\omega}_s|_{k=n} \tag{4.103}
$$

It should be noted that these methods are likely too dependent on the training source data to be used for a general case. However, the observations from studying these models illustrate that the local neighborhood of cells do have enough information to model the subgrid scale effects on the apparent reactivity. This knowledge means that further spatial refinement may not be needed if the surrounding information is used appropriately. Further study is needed to determine if these methods are universal enough to be used for a general case.
4.10.7 Damköhler Extension

An extension based on comparing correlations between the exact LSM model with the LSM-MMD and LSM-FS models for a range of Damköhler numbers was explored. The Damköhler number is defined here as the ratio of subgrid mixing time scale, $\tau_m$, to chemical time scale, $\tau_c$.

$$D_a = \frac{\tau_m}{\tau_c} \quad (4.104)$$

$$\tau_c = \frac{\rho}{||\dot{\omega}||} \quad (4.105)$$

$$\tau_{SGS} = \frac{\Delta}{u_{SGS}} \quad (4.106)$$

The proposed extension to these models was aimed at blending the laminar chemistry source terms with the model-driven source terms by driving the enhancement factor to one for low Damköhler numbers. The proposed blending is given by Eq. 4.107, where $f_m$ is the enhancement factor predicted by either LSM-MMD or LSM-FS.

$$f_{Da} = [1 - \beta(Da)]f_m + \beta(Da)f_{LC} \quad (4.107)$$

Based on a priori analysis (see section 5.1.2), the average $\beta$ corresponds to a constant ($\approx -0.15$) for moderate to large Damköhler numbers for both the LSM-MMD and LSM-FS models. The LSM-MMD model tends to go to one for small Damköhler numbers. The LSM-FS model tends to enhance reactivity for Damköhler numbers near zero. It is found that a quadratic curve can be used to approximate the average $\beta$ function in this region so that a value of one is recovered for $D_a = 0$. Eq. 4.108 defines the extension for the LSM model where the corresponding function for $\beta$ is given by Eq. 4.109. In this work, this model is termed LSM-Damk.

$$\omega_s = \omega_s(\bar{q})$$

$$\bar{\omega}_s = \text{sign}(\omega_s) \left[ (1 - \beta)|\omega_s| + \beta|\dot{\omega}_s| \right] \quad (4.108)$$

$$\beta(D_a) = \begin{cases} 4.6(D_a - 0.5)^2 - 0.15 & \text{if } D_a \leq 0.5 \\ -0.15 & \text{else} \end{cases} \quad (4.109)$$

The extensions presented in Sections 4.10.6 and 4.10.7 provide promising improvements to the baseline LSM models. However, it is important to acknowledge the disadvantage of them. The primary disadvantage is that the models built in these sections were built on a ‘training set’ of data associated with a specific reaction mechanism and a specific combustion process. There is no guarantee that the correlations used in determining the model constants will hold for other cases, particularly in the case of different flame structures. These methods are therefore less general than the other models discussed.
One area of future work is to see if these correlations hold for more general cases; if they do not, development of model extensions that are more general should be pursued.

4.10.8 Further Discussion

Further analysis of the expected action of these models can be done using a Taylor series expansion of the filtering operation (Eq. 4.91). For the purpose of this discussion, a Cartesian grid is assumed and filtering occurs over 27 cells. When applying a 3D filter over a group of 27 uniform cells, there are 6 face neighbors, 12 edge neighbors, and 8 corner neighbors to the center cell \((i, j, k)\). The general filtering operator was given in Eq. 4.91, where the face, edge, and corner neighbors were weighted separately as shown in Table 4.1. Using a Taylor series expansion, the filtering operator can be written in terms of the center cell information. For example, a general variable \(q\) can be approximated at the \(i+1\) neighboring cell as shown in Eq. 4.110. Note that face neighbors only require displacement in one direction.

\[
q_{i+1,j,k} = q_{i,j,k} + \Delta \frac{\partial q}{\partial x} + \frac{\Delta^2}{2} \frac{\partial^2 q}{\partial x^2}
\] (4.110)

Edge neighbors require spatial displacement in two directions. For example, the information at cell \((i+1, j+1, k)\) is approximated as shown in Eq. 4.111.

\[
q_{i+1,j+1,k} = q_{i,j,k} + \Delta \left( \frac{\partial q}{\partial x} + \frac{\partial q}{\partial y} \right) + \frac{\Delta^2}{2} \left( \frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} \right) + \Delta^2 \left( \frac{\partial^2 q}{\partial x \partial y} \right)
\] (4.111)

Finally, the corner neighbors require displacement in all three directions as shown below.

\[
q_{i+1,j+1,k+1} = q_{i,j,k} + \Delta \left( \frac{\partial q}{\partial x} + \frac{\partial q}{\partial y} + \frac{\partial q}{\partial z} \right) + \frac{\Delta^2}{2} \left( \frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} + \frac{\partial^2 q}{\partial z^2} \right)
+ \Delta^2 \left( \frac{\partial^2 q}{\partial x \partial y} + \frac{\partial^2 q}{\partial x \partial z} + \frac{\partial^2 q}{\partial y \partial z} \right)
\] (4.112)

Substituting the expressions analogous to those shown in Eqns. 4.110 through 4.112 for the 26 neighboring cells into the filtering operation, and recognizing that the first derivatives and the mixed second order derivatives of the cells that are symmetric across a directional plane (e.g. cells \(i+1, j,k\) and \(i-1, j,k\) or \(i+1, j+1,k\) and \(i+1, j-1,k\)) cancel one another in the direction of symmetry, Eq. 4.113 can be derived. Eq. 4.113 can be simplified by defining the constant \(C_\alpha = \left(2\alpha_{-2} - 8\alpha_{-19} + 8\alpha_{21-27}\right)/2\).

\[
\hat{\omega}_s = \hat{\omega}_s + \left(2\alpha_{-2} - 8\alpha_{-19} + 8\alpha_{21-27}\right) \frac{\Delta^2}{2} \left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} + \frac{\partial^2 \omega}{\partial z^2} \right)
\] (4.113)

\[
\hat{\omega}_s = \hat{\omega}_s + C_\alpha \Delta^2 \nabla \cdot \nabla(\hat{\omega}_s)
\] (4.114)
The expression in Eq. 4.114 shows that the action of the filtering operation is dependent on the curvature of the function describing the chemical source terms in the local region of the center cell.

Using Eq. 4.114 the formulations for the enhancement factors can be redefined. For example, the LSM-FS model can be redefined as shown in Eq. 4.115. Similarly, the LSM-MMD model can be defined as shown in Eq. 4.116.

\[
\begin{align*}
\tilde{f}_{\text{LSM-FS}} &= \frac{\sum_s \dot{\omega}_s \dot{\omega}_s |1 + C_\alpha \Delta^2 \nabla \cdot \nabla (\dot{\omega}_s) / |\dot{\omega}_s|}{\sum_s \dot{\omega}_s \dot{\omega}_s} \\
\tilde{f}_{\text{LSM-MMD}} &= \frac{\sum_s \dot{\omega}_s \dot{\omega}_s \min \left(1, \frac{|1 + C_\alpha \Delta^2 \nabla \cdot \nabla (\dot{\omega}_s) / |\dot{\omega}_s|}{\sum_s \dot{\omega}_s \dot{\omega}_s}\right)}{\sum_s \dot{\omega}_s \dot{\omega}_s}
\end{align*}
\]

Written this way, the enhancement factor is a function of weighted sums of one plus the ratio of the curvature of the source term to the source term itself. If this ratio is large and the sign of the curvature is opposite that of the source term for a given species, then the LSM-FS model decreases that portion of the weighted sum. If the signs of the curvature and the source term are the same, then the model enhances that part of the sum. The LSM-MMD model does not allow for enhancement to occur. Each species is weighted by the square of their production rate. This means that the models will respond more strongly to the largest source term in the system. This also means that the model will respond to the chemistry; the species that are more active in a particular region of a flame will have the dominant effect on the action of the enhancement factor. Since the LSM models are sensitive to curvature, increasing the resolution of the reaction layer will diminish the effect of the model. For a highly resolved reaction layer, LSM reduces to laminar chemistry.

Further, one must realize that the LSM-based models act on source terms that are defined at specific points in space. Taking a bell curve to represent the production rate of water, one can imagine how the locations of positive curvature can result in increases of low reactivity regions and thus a broadening of the resolved reaction front. The LSM-MMD model will generally not broaden reaction layers due to neglecting the regions with positive curvature to source term ratios. This means that the LSM-MMD model always attenuates and is only applied to the resolved reaction layer. In short, the LSM-FS model will lower peaks and raise valleys of a function that describes the production rates within the reaction layer; LSM-MMD will only lower the peaks. Results portraying these effects are presented in Section 5.1.2.

The LSM-SS model can also be recast in a similar fashion as shown below.

\[
\begin{align*}
\tilde{f}_{\text{LSM-SS}} &= \frac{\sum_s |\dot{\omega}_s (\hat{q})| |\dot{\omega}_s (\hat{q})| |1 + C_\alpha \Delta^2 \nabla \cdot \nabla (\dot{\omega}_s) / |\dot{\omega}_s (\hat{q})|}{\sum_s \dot{\omega}_s (\hat{q}) \dot{\omega}_s (\hat{q})} \\
\end{align*}
\]

Assuming the general, but not universal, premise that |\dot{\omega}_s (\hat{q})| > |\dot{\omega}_s (\hat{q})|, it is clear that the LSM-SS model will be generally attenuating. However, this assumes that the spatial distributions of \dot{\omega}_s (\hat{q}) and
\( \dot{\omega}_s(\hat{q}) \) are similar. This is not necessarily true in the case of premixed flames. Filtering of the flow variables of a poorly resolved premixed flame will result in the distribution of \( \dot{\omega}_s(\hat{q}) \) having a peak value away from the resolved flame front. This results in peak attenuation occurring away from the flame, reducing the effectiveness of the LSM closure model.

All of this discussion still does not directly address how these models account for the effects of unresolved turbulence. One explanation is based on the fact that the turbulence at the mesh scale and below can wrinkle and stretch the flame front which can have an enhancing or diminishing effect on the reactivity. However, due to the implicit LES formulation, this process is spatially averaged over a larger volume based on the mesh scale. The LSM models attempt to model this effect by scaling high-reactivity estimates based on the laminar chemistry assumption by a curvature-dependent factor that is generally less than one. Since laminar chemistry is very likely to provide an overestimate of reactivity, the net result is a reduction in reactivity at locations of high curvature.
Chapter 5

Results and Discussion

5.1 Supersonic Hydrogen-Air Shear Layer

This section discusses the studies of a simplified supersonic combustor represented by a reacting hydrogen-air shear layer. This case has been revisited periodically under different flow conditions to simulate anchored, lifted and triple flame like structures. Two cases will be discussed in this work. The first case is used in the velocity coupling and modified \textit{a priori} analysis. The flow conditions for this case (labeled Case 1) are given in Table 5.1, and are approximate to those in [86]. This case also has a heated boundary layer near the injector wall that has a maximum temperature of \(~1500\)K. This results in a more anchored, diffusion flame where the reactants start burning almost immediately upon mixing. The other variation to this hydrogen-air shear layer will be discussed in section 5.1.3. In both cases, the flow travels in the x-direction as shown in Figure 5.1, with the slot injector extruding in the z-direction. The flame surface is visualized in Figure 5.1 with a \(T=2200\)K iso-surface.

Early in this work, mesh-sequenced realizations were used to assess whether passing of filtered chemical source terms would result in improved simulations on coarser grid levels when compared to a fine grid solution. However, model development has only considered two grid levels up to this point, so only results from these two grid levels will be discussed here. In this thesis, the ‘fine’ and ‘coarse’ grids corresponds to the grid resolutions reported in Table 5.2. The goal is to use fine-grid information to account for the effects of the unresolved turbulent fluctuations on the chemical source terms for a coarser grid resolution. This approach is our ‘modified \textit{a priori}’ analysis, and requires coupling of the velocity fields to ensure that the eddy evolution is highly correlated between grid levels. This will ensure that we are comparing the chemical source terms between grid levels in a meaningful manner.

Both 2D and 3D simulations were conducted early on in the study. Figure 5.2 compares a 3D solution to a 2D solution for the fine grid. Note the decrease in spreading of the 3D solution compared to
the 2D solution, and the corresponding decrease of mixing transverse to the flame surface. This figure demonstrates the need for using 3D simulations in developing the turbulent closure models since turbulent combustion is an inherently 3D process. Although, 2D simulations were used for initial testing and code development, 3D simulations were used to develop, analyze, and test the combustion closure models. All results presented in this work are from 3D simulations.

Table 5.1: Freestream flow conditions for hydrogen-air shear layer (Case 1).

<table>
<thead>
<tr>
<th>Property</th>
<th>Air Stream</th>
<th>Jet Stream</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity (m/s)</td>
<td>1420</td>
<td>1780</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>1250</td>
<td>545</td>
</tr>
<tr>
<td>Pressure (Pa)</td>
<td>107800</td>
<td>107000</td>
</tr>
<tr>
<td>(Y_{H_2})</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>(Y_{H_2O})</td>
<td>0.1730</td>
<td>0.0</td>
</tr>
<tr>
<td>(Y_{O_2})</td>
<td>0.2521</td>
<td>0.0</td>
</tr>
<tr>
<td>(Y_{N_2})</td>
<td>0.5739</td>
<td>0.0</td>
</tr>
</tbody>
</table>

5.1.1 Velocity Coupling

Before an analysis of the reactive chemical source terms can be made, a method for coupling the velocity fields must be defined to ensure that eddy evolution between grid levels is the same. Figure 5.3 shows uncoupled snapshots of the temperature contours of the 3D shear layer case. These simulations were evaluated over the same amount of time, and this snapshot corresponds to the same instance in time for the same starting conditions (with necessary filtering for the coarse grid). Clearly, the structures of the instantaneous flames are different. The coarse grid has a thicker, hotter flame compared to the fine grid and there are noticeable differences in the size and resolution of the distinct eddies. The fine grid resolves some of the smaller structures within the flame while the coarse grid has fewer, larger structures. The flame structure is also slightly wider on the coarse grid due to increased volumetric expansion of the flame. All of this indicates that there is a need to couple the velocity fields between the grid levels to enable comparison of discrete points in space and time.

Table 5.2: Grid resolutions in the isotropic region.

<table>
<thead>
<tr>
<th>Grid Name</th>
<th>(\Delta x)</th>
<th>(\Delta y)</th>
<th>(\Delta z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine Grid</td>
<td>0.4 mm</td>
<td>0.2 mm</td>
<td>0.2 mm</td>
</tr>
<tr>
<td>Coarse Grid</td>
<td>0.8 mm</td>
<td>0.4 mm</td>
<td>0.4 mm</td>
</tr>
</tbody>
</table>
Figure 5.1: Visualization of flame surface for 3D hydrogen-air shear layer.

Figure 5.2: Comparison between 2D (top) and 3D (bottom) solutions for hydrogen-air shear layer.
A method for coupling the velocity fields was discussed in Section 4.9.1. A series of pure mixing simulations were carried out to compare the results with and without coupling to ensure that the velocity coupling resulted in appropriate mixing and eddy evolution. One coarse grid was coupled with the fine grid, while the other coarse grid had no fine grid information. Time-averaged statistics were compared for these cases to determine if the velocity coupling method provided an improved mixing solution. Simply plotting the time-averaged contour plots does not provide sufficient distinction between solutions to assess whether the coarse grid is improved. Instead, the domain was spatially averaged in the z-direction to provide an ensemble average in the x-y plane. Statistics were then processed at four different x-locations, as given by Table 5.3, measured from the injector lip.

Table 5.3: Approximate planar x locations of data points for analyzing statistics.

<table>
<thead>
<tr>
<th>Station</th>
<th>x coordinate (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.015</td>
</tr>
<tr>
<td>2</td>
<td>0.041</td>
</tr>
<tr>
<td>3</td>
<td>0.128</td>
</tr>
<tr>
<td>4</td>
<td>0.224</td>
</tr>
</tbody>
</table>
Mean flow variables are plotted at two of these stations as shown in Figures 5.4 - 5.9 for the simulations using the PPM scheme with Ducros. Figures 5.4 and 5.5 clearly show that coupling results in almost exact matching of mean velocity profiles with that of the fine-mesh result. Mixing also appears to be improved as observed in the density, temperature, and hydrogen mole fraction plots, which show better agreement between the coupled and fine grid profiles relative to the uncoupled case.

Given that our coupling of the velocity fields results highly correlated instantaneous eddy structures as well as mixing solutions that match more closely with fine-mesh statistics, we can build a database of temporal and spatial points for conducting a modified a priori analysis. The database is built by dumping the field variables at discrete locations from the coupled 3D reacting shear layer. The results from this analysis and the various methods for assessing the different models are discussed in the next section.
Figure 5.4: Comparisons of mean U velocity profiles for mixing shear layer.

Figure 5.5: Comparisons of mean V velocity profiles for mixing shear layer.
Figure 5.6: Comparisons of mean density profiles for mixing shear layer.

Figure 5.7: Comparisons of temperature profiles for mixing shear layer.
Figure 5.8: Comparisons of mean pressure profiles for mixing shear layer.

Figure 5.9: Comparisons of hydrogen mole fraction profiles for mixing shear layer.
5.1.2 Results: Modified \textit{a priori} Analysis

The concept of a modified \textit{a priori} analysis was discussed in Section 4.9.2. In this section, the results of this analysis is discussed. The database of points used in the modified \textit{a priori} analysis consists of 2500 discrete locations at five different planes along the x-direction. The locations of these planes are given by Table 5.4. These coordinates are measured from the injector lip and are shown in Figure 5.10. Data was written at 31,500 discrete points in time, corresponding to approximately 0.5 milliseconds or five combustor transit times (CTTs). The data written included all species densities, the three components of the velocity vector, temperature, mixture density, and pressure as well as cell volume and physical time. For every coarse grid cell to be written, the data from the eight fine grid cells corresponding to the coarse grid cell is written. Data from the 26 neighboring cells, on the coarse grid, are also written. This will allow numerous additional quantities and filtering operations to be explored in the \textit{a priori} analysis.

<table>
<thead>
<tr>
<th>Station</th>
<th>x coordinate (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>0.05</td>
</tr>
<tr>
<td>3</td>
<td>0.10</td>
</tr>
<tr>
<td>4</td>
<td>0.15</td>
</tr>
<tr>
<td>5</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Using this data, there are several ways that we can visualize and predict the effects of the different models proposed. Perhaps the simplest method for assessing the models is to plot the model numerator predictions versus the exact numerator. The effect on individual source terms, heat release or norm of the chemical source term vector can also be compared. Probability density functions of the ratio of these reactivity measures to the fine grid information as well as the enhancement factors have also been generated to assess the models. Also falling out of this analysis are some correlations between calculable flow parameters and the exact enhancement factor averaged over a large sample of the data points. These methods will be discussed throughout this section as well as some of the conclusions drawn from the analysis.

The most straightforward approach in comparing these models is to plot the model numerators from Eq. 4.89 versus that of the exact model. This is shown in Figure 5.11 which compares the model numerators of the LSM-FS model for two different filter widths versus the exact LSM model and the laminar chemistry equivalent. The scatter data shown includes all but the first station of data points.
Figure 5.10: Locations of \textit{a priori} data points in space.
The desired result is a slope of unity with little to no scatter. Therefore, it appears that a filter width of twice the mesh scale is slightly more preferable for the LSM-FS model since the correlation and slope are slightly better than the case of $1\Delta$. Similarly, Figure 5.12 compares the LSM-FS-H model for two different filter widths versus the exact and laminar chemistry equivalents with heat included. Note that the axis scales are different between Figures 5.11 and 5.12 due to the inclusion of the heat release which adds to the magnitude. Figure 5.12 indicates that a filter width equal to twice the mesh scale is preferable when heat release is included. Both figures show that both models result in some decrease in scatter and slope compared to laminar chemistry.

From this analysis it can also be shown that there exists a single point in the neighborhood of 27 cells that collapses the scatter observed for the LSM-FS models. Figure 5.13 shows the model numerators for Eq. 4.100 which uses the optimal cell on the coarse grid to evaluate the LSM model numerator. This optimal cell is the cell that minimizes the difference in the source term for water and the source term filtered from the fine grid. Using this single point results in a large reduction in the scatter and a slope very close to one. Several methods for trying to predict this cell based on information on the coarse grid level have been investigated. One attempt involved using artificial neural networks available in software packages such as Matlab and JMP-Pro to model a function for the difference in the source term of water for each cell neighboring the cell for which the model is being applied and the filtered fine grid source.
of water for that cell. One such model results in the scatter plot shown in Figure 5.14. A decrease in scatter is observed, but the slope is less, meaning that the model numerators under predict those of the exact model.

While plotting the x-y scatter plots offers some indication what a model might do compared to laminar chemistry, it provides no indication of the effect of the model over the spatial domain. Figure 5.15 shows a comparison of model numerators for the cases of the exact LSM, LSM-FS, LSM-JMPANN, and the LC equivalent in the x-y plane. The model numerators are plotted in the z-direction with the points being colored based on the numerator value. Two important observations come from this figure. The exact model shows significantly more attenuation at the first two stations compared to laminar chemistry than at the last three stations. This is because the first station corresponds to the ignition location on the coarse grid while the solution obtained on the fine grid is not actually burning at that location. It is also noted that the LSM-FS model actually attenuates slightly more at the last three stations than the exact model. The JMP-ANN model appears to attenuate much more at the first two stations compared to LSM-FS, and doesn’t attenuate as much at the third station.

Another method used to assess the models is to plot the corrected source terms or heat release values versus the fine filtered values and the laminar chemistry values directly for comparison. For example, Figure 5.16 and 5.17 compare the effect of including the heat terms on the water production rate and model heat release, respectively. An important observation is that including the heat term in the model...
Figure 5.13: Comparison of optimal single point numerator with exact numerator.

Figure 5.14: Comparison of JMP-ANN predicted numerator with exact numerator.
Figure 5.15: Comparison of model numerators over flow domain.
formulation doesn’t appear to have much effect on the modeling of the water source term, but does collapse the heat release to match more closely with the fine-mesh heat release. Figure 5.17 also shows that, although it attenuates the source terms of water, the exact LSM model does not correct the heat release significantly.

![Figure 5.16: Effect of the inclusion of heat on modeled water production rate.](image)

Figure 5.18 shows the probability density function for the ratios of filtered fine grid sources to coarse grid sources using different closure models. Data points within the mixture fraction range of \( Z = Z_{st} \pm 0.02 \) from all but the first station were used in generating these PDFs (\( Z_{st} \approx 0.0298 \) for hydrogen-air flames). The desired result is a narrowing of the PDF near a value of one, as nearly achieved by the exact LSM model. The laminar chemistry result on the coarse grid shows that it is highly probable that the coarse grid will over-estimate reactivity since the peak of the PDF is in the range between zero

80
Figure 5.17: Effect of the inclusion of heat on modeled heat release.
and one. Results from the LSM-FS and LSM-MMD models are displayed in Figure 5.18 as well, and while they do not narrow the PDF, both models result in a shift in the peak closer to one. It is also noted that the PDFs for the LSM-FS and LSM-MMD models are very similar, despite the fact that LSM-MMD does not allow for enhancement. Further, it is observed that there is a chance that there is a sign difference between the fine-filtered production rates and the coarse grid source terms. These points are less probable, and they likely exist in regions very close to equilibrium or at significantly high temperatures where some dissociation of water is occurring on one grid or the other. The probability of water dissociation is increased due to the high water concentration in the air co-flow. These PDFs do not indicate that a negative enhancement factor will be predicted on the coarse grid; the LSM models are specifically formulated to not allow for a negative enhancement factor as discussed earlier.

Figure 5.18: PDFs of the ratio of chemical source terms for different closure models.

Figure 5.19 compares the PDFs of chemical source term ratios for closure models that include heat release in their formulation including the LSM-FS-H and LSM-SS-H models. The exact model with heat release, again, results in the desired result with the peak value shifting to unity and a narrowing of the PDF. However, it is noted that the probability of a ratio of unity is actually lower than when heat release is not included, at least for the source terms shown here. This is because the inclusion of heat release adds additional weighting to species with larger heats of formation. Again, all closure models improve over laminar chemistry by shifting the PDF toward one. It is also noted that although the LSM-SS-H model uses a smaller filter width, it still results in higher likelihood of decreasing the reactivity more
than predicted by the LSM-FS-H model.

Figure 5.19: PDFs of the ratio of chemical source terms for different closure models that include heat.

The ratio of heat release for different closure models is also compared as shown in Figure 5.20. Models that do not incorporate heat release are shown on the left while models with heat are on the right. Clearly, incorporating heat release results in better agreement with the fine grid heat release as shown by comparing the LSM-FS and LSM-FS-H or exact and exact-H models. Also shown is the LSM-MMD model which again is similar to the LSM-FS model. The ratio of the LSM-SS-H model is shown in the right figure and results in a PDF that indicates more attenuation of heat release.

Finally, Figure 5.21 compares the enhancement factors for the same models as shown in Figure 5.20. The LSM-FS and LSM-MMD models are very similar except that the LSM-MMD model does not allow for augmentation of reactivity. The LSM-SS-H model is significantly more likely to predict enhancement factors near zero compared to the other models. It is also noted that the exact model with heat shows higher probability of augmentation that the LSM-FS-H model.

Another goal of this modified \textit{a priori} analysis is to seek correlations between the exact models and other quantities including Damköhler number and mixture fraction. One extension builds on the idea of the ‘optimal single point,’ for use in Eq. 4.100, and correlations that could be used to predict this point were investigated. One idea in order to try and seek these correlations is to consider a local
Figure 5.20: PDFs of the ratio of heat release for different closure models.

Figure 5.21: PDFs of enhancement factors for different closure models.
neighborhood of cells and define a reduced reactivity measure, \( R_k \).

\[
R_k = \frac{||\dot{\omega}\||_k - ||\dot{\omega}\||_{\min}}{||\dot{\omega}\||_{\max} - ||\dot{\omega}\||_{\min}}
\]  

(5.1)

The cell in the neighborhood that is found to be the ‘optimal’ cell is defined as cell \( k = M \). This gives a convenient parameter (varying between zero and one) to average and analyze for every cell. A \( R_M \) value of one indicates that maximum local reactivity is optimal while a value of zero indicates that the minimum local reactivity is optimal. Taking a large subset of the data, the PDF for the value \( R_M \) was generated as shown in Figure 5.22. This shows that there is almost no probability of the maximum local reactivity being the optimal measure for providing closure for the source terms. Instead, the local minimum reactivity is the most probable. The curve shown in the figure is an exponential curve that can be used to describe the range of \( R_M \) from 0.2 - 1.

Figure 5.22: PDF of \( R_M \) value.

One option to use this information is to simply use a constant value that is highly probable (e.g. \( R_M = 0.1 \)). Another option is to see if a value for \( R_M \) can be predicted based on some other variable that obeys the PDF. In attempting to model \( R_M \), the fits in Figure 5.23 were generated. On the left, a fit for the average \( R_M \) as a function of mixture fraction is created using two cubic functions. On the right, is a linear fit for the average \( R_M \) as a function of local Damköhler number. Noting that some scatter is present, some interesting trends are observed. First, for rising Damköhler number, a lower \( R_M \) value is predicted. This trend correlates with the observation that for increasing turbulent time scale (increasing Damköhler number for constant chemical time scale) laminar chemistry will likely over-predict chemical reactivity.
due to insufficient mixing by the turbulent fluctuations that are occurring. It also makes sense that the value of $R_M$ for low Damköhler number should be somewhere in between zero and one since, if turbulent mixing is very intense or chemistry is very slow, laminar chemistry may be appropriate. When observing the trends relative to mixture fraction, other observations can be made. First, only points near stoichiometric mixture fraction ($Z_{st} \approx 0.0298$) are likely to be meaningful, because probability of reactions occurring decreases rapidly as conditions move away from the stoichiometric value. This explains the increase in scatter for mixture fractions further away from stoichiometry. Focusing on the range $Z = [0, 0.06]$, it is observed that much more attenuation is observed on the oxidizer side compared to the fuel side. In fact, based on our PDFs and observations regarding Damköhler number, it is possible that enhancement could occur on the fuel-rich side of the stoichiometric curve. It should be noted that this response may be case-specific, and further analysis is needed to determine otherwise.

Finally, an extension to the LSM-FS and LSM-MMD based on correlations with Damköhler number is defined, which blends the model predictions with laminar chemistry. Figure 5.24 shows average enhancement factor values for given Damköhler number; the exact LSM, LSM-FS, and LSM-MMD models are compared. The averages were taken over all stations except for the first station. This figure shows that there is a clear correlation between increasing local Damköhler number and increasing level of attenuation. The LSM-FS and LSM-MMD models both result the same averages for Damköhler numbers of 0.5 or higher, but do not attenuate as much as the exact model. For low Damköhler numbers, the models appear to attenuate more than the exact model. Given that low Damköhler numbers correspond to the ‘well stirred’ reactor regime, laminar chemistry may be appropriate. This leads to the formulation
of a model extension that blends the model enhancement factor with laminar chemistry at low Damköhler numbers and provides a correction that matches more closely with the response of the exact model at higher Damköhler numbers.

Figure 5.24: Average enhancement factor vs Damköhler number for exact, LSM-FS, and LSM-MMD models.

The formulation for this Damköhler based model extension was given in section 4.10.7, where $\beta$ is modeled by Damköhler number. In order to seek correlations for $\beta$, Eq. 4.107 was rearranged to obtain an expression for $\beta$, taking advantage of the fact that $f_{LC} = 1$. Here $f_m$ is the enhancement factor predicted by the LSM-FS or LSM-MMD models.

$$\beta = \frac{f_{DA} - f_m}{1 - f_m} \quad (5.2)$$

Correlations for $\beta$ are sought by defining $f_{DA}$ in Eq. 5.2 as equal to the exact LSM enhancement factor and averaging the corresponding values of $\beta$ for a given Damköhler number. The result of this process is shown in Figure 5.25. Although there is some scatter to the figure, it is clear that a roughly constant value of average $\beta$ is obtained for $D_a > 0.5$ for both the LSM-FS and LSM-MMD models. This value is approximately -0.15. In the range of low Damköhler number, a quadratic curve can be used to drive the value for $\beta$ to one so that laminar chemistry is recovered for low Damköhler number. Again, it is
noted that, although this analysis shows a correlation between the optimal value of the enhancement factor and Damköhler number exists, the specific functional form may be case-specific. Further analysis is required to determine the universality of the response.

![Figure 5.25: Average $\beta$ value vs Damköhler number for $f_{Da} = f_{exact}$.](image)

As discussed in Section 4.10.8, the action of the LSM-FS and LSM-MMD models depend on the curvature of the chemical production rate distributions. This is illustrated in Figure 5.26 which shows conditional averages of different production rates for given mixture fractions at the second station. This station corresponds to the most reactive station on the fine grid. The coarse-grid results overestimate each of the chemical source terms relative to the fine-grid prediction using laminar chemistry. The LSM-FS and LSM-MMD source terms are also shown. Note that both reduce the peaks of each curve. Also observed is that the LSM-MMD model prediction is consistently lower or equal to the laminar chemistry prediction on the coarse grid due to the limiting behavior of the model. The LSM-FS model shows some enhancement relative to laminar chemistry where the curvature and source term signs match. Figures 5.27 through 5.29 show conditional averages at stations 3-5, which are further downstream. The axis scales for these figures are different from Figure 5.26 since Station 2 is much more reactive. It is noted that as the observer moves downstream, a decrease in reactivity is observed along with better agreement between laminar chemistry predictions between grid levels. By Station 5, all models are relatively close to one another; however, reactivity is very low as the flame is reaching equilibrium.
Figure 5.26: Conditional averages of species production rates versus mixture fraction for Station 2.
Figure 5.27: Conditional averages of species production rates versus mixture fraction for Station 3.
Figure 5.28: Conditional averages of species production rates versus mixture fraction for Station 4.
Figure 5.29: Conditional averages of species production rates versus mixture fraction for Station 5.
5.1.3 Model Testing

Before implementing the models in one of the expensive application simulations, the models were tested for the reactive shear layer case. This allows multiple simulations at multiple grid levels to compare the effects of the models. This analysis is used to get a quick idea of which model might be best for further testing. For this testing, the modified solver (discussed in Section 4.9.1) is used again to run simulations on the fine grid along with up to five coarse grids that each may implement a different model. Comparisons can then be made between a fine grid solution along with coarse grid solutions using laminar chemistry and any other closure models that are promising. In this section, time averaged results will be compared for various closure models for two different run conditions corresponding to a reacting hydrogen shear layer. The first, referred to as Case 1, is under the conditions given in Table 5.1. The second, Case 2, is governed by the conditions in Table 5.5. Between cases there are changes in composition, temperature, and jet stream speed. Case 2 now has a pure air co-flow and a jet that is sonic rather than entering at Mach 2. Another difference between these two cases is that Case 2 does not have a heated boundary layer along the injector wall. The numerics between cases are the same, both using PPM with Ducros switch. Coarse and fine grid solutions were compared for Case 1 in Figure 5.3. The coarse and fine grid solutions for Case 2 are compared in Figure 5.30.

Table 5.5: Freestream flow conditions for hydrogen-air shear layer (Case 2).

<table>
<thead>
<tr>
<th>Property</th>
<th>Air Stream</th>
<th>Jet Stream</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity (m/s)</td>
<td>1420</td>
<td>890</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>1300</td>
<td>545</td>
</tr>
<tr>
<td>Pressure (Pa)</td>
<td>107800</td>
<td>107000</td>
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<tr>
<td>$Y_{H_2}$</td>
<td>0.0</td>
<td>1.0</td>
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<tr>
<td>$Y_{H_2O}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$Y_{O_2}$</td>
<td>0.24</td>
<td>0.0</td>
</tr>
<tr>
<td>$Y_{N_2}$</td>
<td>0.76</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Before discussing the time averaged results, some general observations on the two cases will be made. For Case 1, the laminar chemistry solutions on both grids appear very similar to each other. There is no change in the basic flame structure; both flames are anchored fairly close to the injector and have nominal mixing transverse to the flame, relying on turbulent and molecular diffusion to feed the flame. The primary differences are that the coarse grid flame is generally thicker and hotter compared to the fine grid flame. The ignition point is slightly further upstream compared to the fine grid. For the second case, the two solutions are quite different. First, the fine grid flame is much more lifted and appears to be more of a triple flame than a pure diffusion flame. The level of transverse mixing is much higher in this
Figure 5.30: Comparison of snapshots of temperature between grid levels for Case 2.

Figure 5.31: Comparison of snapshots of pressure between grid levels for Case 2.
case as well, with hot products mixing into the centerline of the domain, unlike the first case. Also, as shown in Figure 5.31, the compression wave due to the expansion of the flame is much stronger on the fine grid compared to the coarse grid. This gives us two very different cases for which comparisons can be made. In Case 1, the desired effect of the model would be to simply attenuate the flame temperatures and possibly shift the ignition point downstream. For Case 2, the successful model would account for the different flame structures, ideally by delaying ignition and allowing more mixing to occur before reactions begin. This should result in a more sudden ignition and a stronger compression wave.

Starting with Case 1, time averaged solutions for the fine grid and coarse grid with laminar chemistry are shown in Figure 5.32. Figure 5.32 simply supports the fact that solutions between grid levels for Case 1 are very similar relative to Case 2. The observations made previously based on instantaneous snapshots are further supported by this figure in which the temperature of the flame is hotter on the coarse grid compared to the fine grid as well as being thicker. The pressure fields are also very similar with the compression wave being slightly closer to the injector due to the ignition point being closer.

![Figure 5.32: Average temperature and pressure for coarse (top) and fine filtered (bottom) solutions for Case 1.](image)

The effects of various closure models are compared in Figures 5.33 through 5.36 in which time-averaged statistics of temperature, pressure, density, and water mole fraction are shown at stations 2 and 4 (see Table 5.3 for x locations). As was mentioned previously, the solutions between fine and coarse grids using laminar chemistry are already very close. The primary differences are the location at which the flame begins to burn, the peak temperatures and the degree of flame expansion. The coarse grid with laminar chemistry begins to ignite closer to the injector and expands further with higher peak
temperatures by the exit of the domain. The models compared here are the LSM-FS model along with a model for predicting $R_M$ by a linear fit for Damköhler number, termed Da-MMD, and by setting $R_M = 0.1$. See Figure 5.23 for the trends relating Damköhler number and $R_M$. These optimal single point models are combined with the MMD approach to ensure no enhancement of reactivity occur. Examining the results, it is noted that the only major change observed is a shift in the location of the ignition point. In order of increasing displacement, the LSM-FS, $R_M = 0.1$, and Da-MMD models all result in moving the ignition location downstream of that predicted by laminar chemistry. However, by the fourth station, all results on the coarse grid are nearly the same for all variables. The LSM-FS and $R_M = 0.1$ models result in better matching of the mean pressure field with the fine grid at the second station as well, because of the change in shock position.

Figures 5.37 and 5.38 compare contour plots of the fine filtered and coarse grid solutions using laminar chemistry and the $R_M = 0.1$ models. The $R_M = 0.1$ model is shown here since it results in the best match of ignition location with the fine grid of the models discussed. However, all three closure models resulted in solutions very similar to each other, with very small changes compared to laminar chemistry. The primary change due to implementation of the model closure is a shift of the compression wave, due to ignition of the flame, to a location similar to that predicted by the fine grid. This is more easily observed by the mean pressure contours. The species mass fractions appear to be relatively unchanged compared to laminar chemistry.
Figure 5.34: Comparisons of temperature statistics for Case 1 using various closure models.

Figure 5.35: Comparisons of mean pressure for Case 1 using various closure models.
Instantaneous comparisons between temperature predictions using LSM-FS are compared with predictions using laminar chemistry on the coarse- and fine-grids in Figure 5.39. For this case, it is difficult to identify differences between the two coarse-grid simulations. There are slightly cooler temperatures in the ignition region when using LSM-FS relative to laminar chemistry. There also appear to be some cooler eddies that break up the continuous diffusion flame shown on the coarse grid using laminar chemistry.

For the second case, time-averaged solutions for the fine grid and coarse grid with laminar chemistry are shown in Figure 5.40. As shown in the figure, the flame is more lifted in this case, so comparisons will be made at stations 3 and 4. Note that station 3 corresponds to a location just downstream of the fine grid ignition point. Clearly, the flame structures are quite different between grid levels. The fine-grid solution is characterized by a triple flame like structure while the coarse-grid solution is a turbulent diffusion flame. The fine-grid solution also has stronger expansion and compression waves as well. Constrained and unconstrained solutions will be compared for this case.

Figures 5.41 - 5.44 compare time-averaged statistics for density, temperature, pressure, and water mole fraction, respectively, for the case of a coarse-grid solution constrained by the fine-mesh velocity field. Here laminar chemistry, LSM-FS, LSM-SS-H, and LSM-MMD models are being compared. At station 3, the temperature is matched with the fine grid for the LSM-FS model; however, at the fourth station laminar chemistry matches the fine grid best. Applying a closure model other than laminar chemistry also appears to improve density predictions at both stations. The trend in water mole fraction is the
Figure 5.37: Average temperature and pressure for $R_M=0.1$ - MMD (top), laminar chemistry (middle) and fine filtered (bottom) solutions.

Figure 5.38: Average species mass fraction for $R_M=0.1$ - MMD (top), laminar chemistry (middle) and fine filtered (bottom) solutions.
Figure 5.39: Instantaneous comparison of coarse grid simulations using LSM-FS (top) and LC (middle) versus fine-grid data (bottom) for Case 1.
same as temperature, with laminar chemistry resulting in the best match with the fine grid for the fourth station and LSM-FS being best at station 3.

Figures 5.45 - 5.48 compare mean density, temperature, pressure, and water mole fraction, respectively, for the unconstrained solutions. Looking at Figure 5.46, it is noted that the flame temperatures are cooler for all coarse grid models compared to the fine grid. As we have observed, the closure models selected here attenuate temperature compared to laminar chemistry. Comparing the plots of density and pressure, it is observed that the models result in increased compression in the air density and pressure, with LSM-SS-H resulting in the most compression. So the model closure appears to help attenuate reactivity to the point that ignition is delayed to allow more mixing and push the ignition point downstream. However, the downside is that the temperature has been decreased to a degree that does not match the filtered-fine grid results.

Based on the results of the constrained and un-constrained analysis it seems that some of the large error in predictions on the coarse grid comes from errors associated with mixing rather than chemistry. This is based on the fact that the coarse-grid flame begins burning earlier but is still cooler than the fine-grid. Since these flame structures are quite different between grid levels, it is useful to compare contour plots of the time averaged solutions. Figures 5.49 and 5.50 compare some of the average variables for the LSM-SS-H, laminar chemistry, and fine filtered cases. The LSM-SS-H model was chosen for comparison as it resulted in the most noticeable change in ignition location and pressure. The LSM-
Figure 5.41: Comparisons of mean density for Case 2 using various closure models (constrained).

Figure 5.42: Comparisons of temperature statistics for Case 2 using various closure models (constrained).
Figure 5.43: Comparisons of mean pressure for Case 2 using various closure models (constrained).

Figure 5.44: Comparisons of mean water mole fraction for Case 2 using various closure models (constrained).
Figure 5.45: Comparisons of mean density for Case 2 using various closure models.

Figure 5.46: Comparisons of temperature statistics for Case 2 using various closure models.
Figure 5.47: Comparisons of mean pressure for Case 2 using various closure models.

Figure 5.48: Comparisons of mean water mole fraction for Case 2 using various closure models.
SS-H model seems to improve the solution in some aspects, such as delaying the ignition and thus resulting in a stronger compression effect further downstream, but the flame is still too cool by the exit of the domain. The flame structure also begins to resemble more of a premixed or triple flame similar to the fine grid. Although not compared in the line plots, the composition of the flame is also improved to some degree when a closure model is used. The coarse grid overestimates the water mass fraction and underestimates hydroxyl mass fraction. The LSM-SS-H model results in predictions somewhere in between the laminar chemistry and fine grid predictions for these mass fractions. Both the LSM-SS and LSM-MMD models result in some of the same changes. However, the scale-similarity model resulted in the most change, the most interesting of which, was the moving of the ignition location downstream and the resulting triple flame like structure.

Instantaneous snapshots of Case 2 predictions are compared in Figure 5.51. Again, the LSM-FS model predictions for temperature are compared against laminar chemistry on the coarse- and fine-grids. Here, cooler temperatures are observed when using the LSM-FS model as well as a slight delay in ignition relative to laminar chemistry. In the instantaneous snapshot, the temperatures on the coarse-grid using LSM-FS appear to be closer to the fine-grid data relative to laminar chemistry; however, time-averaged data shows otherwise.

Finally, instantaneous comparisons of model enhancement factor for the LSM-FS model are compared for the two shear layer cases in Figure 5.52. Both show some enhancement of reactivity near the ignition location followed by mostly attenuation downstream of the flame ignition point. The first case has a much thinner region of model activity due to less mixing in the transverse direction.
Figure 5.49: Average temperature and pressure for LSM-SS-H (top), laminar chemistry (middle) and fine filtered (bottom) solutions.

Figure 5.50: Average species mass fraction for LSM-SS-H (top), laminar chemistry (middle) and fine filtered (bottom) solutions.
Figure 5.51: Instantaneous comparison of coarse grid simulations using LSM-FS (top) and LC (middle) versus fine-grid data (bottom) for Case 2.
Figure 5.52: Comparison of instantaneous enhancement factor contours predicted by LSM-FS.
5.2 Model *a posteriori* Testing

This section summarizes and discusses a series of *a posteriori* tests in which the LSM-FS closure model is applied to three cases for which experimental data and results from previous simulations are available. Several other LSM models are also tested and compared for one of these cases. These cases correspond to a series of experiments conducted at the University of Virginia (UVa). A general schematic of the experimental setup at UVa’s supersonic combustion facility (SCF) is given in Figure 5.53 with the combustor test section shown in the zoomed-in view. In this work, the experiments considered were conducted on three flow path arrangements named configuration A, C, and E. These configurations are described by the schematics shown in Figures 5.54, 5.55, and 5.56, respectively. Both configurations A and C have a compression ramp with an injector that marks the entrance of the combustor, while configuration E utilizes a cavity flameholder. The fuel used in configurations A and C is hydrogen, while ethylene is used for configuration E. These cases will be discussed in further detail in the individual subsections along with comparisons of simulation results.

![Figure 5.53: Layout of UVa supersonic combustion facility (SCF).](image-url)

Figure 5.53: Layout of UVa supersonic combustion facility (SCF).
Figure 5.54: SCF configuration A ‘side’ view (top) and ‘top’ view (bottom).
Figure 5.55: SCF configuration C ‘side’ view (top) and ‘top’ view (bottom).

Figure 5.56: SCF configuration E ‘side’ view (top), ‘top’ view (middle), and zoomed view of combustor section (bottom).
5.2.1 Configuration-A

The first case investigated for testing the LSM-FS model corresponds to the scramjet combustion experiment configuration A. The conditions of this case are summarized in Table 5.6; the flow conditions also correspond to that of configuration C. Experimental data for this case includes three-component stereo planar laser velocimetry (PIV), coherent anti-Stokes Raman spectroscopy (CARS), focused Schlieren imaging, OH planar laser induced fluorescence (OH-PLIF), and low-frequency wall pressure measurements. Details of the experiment can be found in [87–89] while detailed analysis of simulations of this experiment using laminar chemistry and a ~33 M cell mesh can be found in [2, 38]. A subsequent study [48] examined the effects of closure models for the effects of turbulent fluctuations on chemical source terms. It is important to note that there is noticeable asymmetry in this flow (as well as configuration C) due to the inlet boundary conditions that model the asymmetric nozzle exit conditions observed in the experiment cited in [90]. Figure 5.57 shows a centerline slice of the flow. Note that the flame is anchored by a low momentum region near the injector due to recirculation behind the ramp.

Table 5.6: Flow conditions for configurations A and C.

<p>| | |</p>
<table>
<thead>
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<tbody>
<tr>
<td>Inflow Mach</td>
<td>2.0</td>
</tr>
<tr>
<td>Inflow temperature (K)</td>
<td>667</td>
</tr>
<tr>
<td>Inflow pressure (kPa)</td>
<td>38.4</td>
</tr>
<tr>
<td>Fuel Mach</td>
<td>1.6</td>
</tr>
<tr>
<td>Fuel temperature (K)</td>
<td>298</td>
</tr>
<tr>
<td>Equivalence ratio</td>
<td>( \phi = 0.17 )</td>
</tr>
</tbody>
</table>

In this work, comparison with the mean and \textit{rms} temperature and species mole fractions is of primary interest. The LSM-FS model was implemented and the calculation initialized from an existing solution obtained as part of the study in [48]. The simulation was evolved for two combustor transit times (CTTs) to wash out transient effects due to model change; statistics were then collected over four CTTs. The transit time is defined as that required for a fluid particle to travel the length of the combustor (0.365 m) while moving at the inflow velocity (1065 m/s). The following analysis will compare the mean and standard deviation for different flow variables obtained from the experimental CARS data along with LES/RANS results using laminar chemistry and the LSM-FS model. The CARS data for this case is available at locations \( x/H = 6, 12, \) and 18 measured from the lip of the injector plane, where \( H \) is the height of the wedge (0.25 inches or 6.35 mm). As the CARS data is scattered within a given plane, the figures were created by interpolating solution data to the CARS data locations. The contour maps were created using the triangulation and Kriging interpolation functions in Tecplot. Included with the contour maps is an outline of the actual physical domain.
Figures 5.58 through 5.63 compare mean and standard deviation of temperature along with mole fractions of hydrogen and oxygen. Improvement in the statistics of temperature are observed in Figures 5.58 and 5.59. The mean temperatures are slightly lower at the last two stations compared to the simulation with laminar chemistry. Also, the flame is developing more along the top wall at the first station when using the LSM-FS model in accord with the experiment. The standard deviations of temperature are also improved for the last two stations when the LSM-FS model is used. An improvement in mean hydrogen mole fraction is also observed at the first two stations when compared with the experimental CARS measurements. The simulation with laminar chemistry shows a high concentration of hydrogen near the top wall indicating that the flame hasn’t developed in this region while both the experiment and LSM-FS model show that the hydrogen is being consumed in this region. Standard deviation of species mole fraction also match more closely to the CARS measurements for the last two stations for the LSM-FS model.

The mean enhancement factor is shown in Figure 5.64 at each of the three stations. The LSM-FS model allows for some enhancement along the outer edges of the flame at the first two stations while attenuating within the hot regions of the flame. By the last station, the LSM-FS model is only attenuating the chemical source terms with values near 0.75, which results in lower temperatures matching more closely with the experiment. Based on these observations, the LSM-FS model appears to attenuate in regions of high reactivity, while enhancing reactivity in high strain regions near the edge of the developing flame.
Figure 5.58: Comparison of mean temperature for configuration A.

Figure 5.59: Comparison of $rms$ temperature for configuration A.
Figure 5.60: Comparison of mean hydrogen mole fraction for configuration A.

Figure 5.61: Comparison of \( \text{rms} \) hydrogen mole fraction for configuration A.
Figure 5.62: Comparison of mean oxygen mole fraction for configuration A.

Figure 5.63: Comparison of $rms$ oxygen mole fraction for configuration A.
5.2.2 Configuration-C

Configuration C is very similar to the setup for configuration A. This case is also hydrogen burning ($\phi = 0.17$) with the same wedge-shaped ramp injector and combustor geometry. The flow domain is modified to include a longer isolator as well as a straight section downstream of the combustor, followed by an extender. Due to the larger geometry, the mesh required for this case is much larger at ~66 M cells. The results shown here were initiated using a laminar chemistry flow solution discussed in [2]. For this case, experimental CARS data was obtained at locations x/H=6, 18, 38, and 56, measured from the lip of the injector plane. Note that the first two stations correspond to the first and third stations of configuration A. The procedure for taking statistics was also the same, with 2 CTTs to remove initial transients and 4 CTTs to collect statistics. Further, the same procedure for interpolating and comparing data points with the experiment was also the same; although, this experiment had a larger number of points for each experimental CARS plane. An instantaneous temperature snapshot of the combustor is shown in Figure 5.65, along with the locations of the CARS stations.

Figures 5.66 - 5.71 compare time-averaged statistics of temperature at four stations for configuration C over three sets of cases. Each set consists of three different simulations using different closure models along with CARS experimental data for comparison. The closure models compared for each ‘case set’ is given in Table 5.7, where each set always compares with laminar chemistry. Time averaged statistics of nitrogen, hydrogen, and oxygen mole fractions are included for reference in Appendix B.1.

Case set 1 compares laminar chemistry results with simulation results using the LSM-FS and LSM-FS-H models along with the experimental CARS data. The mean temperatures are compared in Figure 5.66. Clearly the experimental CARS measurements show cooler flame temperatures than is predicted by any of the three simulations. However, the temperatures predicted using the LSM-FS and LSM-FS-H models appear to be slightly cooler compared to those obtained when using laminar chemistry. The
LSM-FS results appear to have the coolest temperatures of the three simulations, especially at the second and third stations. Comparing the standard deviation of temperatures in Figure 5.67, some decrease is observed when the LSM-FS model is incorporated, which matches more closely with the experiment. The LSM-FS-H model appears to result in standard deviations somewhere in between LSM-FS and laminar chemistry.

The second set of cases compares the JMP-ANN model along with LSM-FS again. The JMP-ANN model results in cooler temperatures at the first station, where the LSM-FS and LSM-FS-H models resulted in mean temperatures unchanged from the laminar chemistry case. The JMP-ANN model, however, results in a hotter flame that has not spread as far into the center of the domain at the second station. While this spatial size of the flame is more consistent with the experiment, the hotter temperatures are not. The third and fourth stations have mean temperatures that actually seem slightly cooler than the experiment. Viewing the mean hydrogen mole fraction in Figure B.11, it is observed that the JMP-ANN model results in more burning of the hydrogen for the last three stations compared to LSM-FS or laminar chemistry. It is also noted that the JMP-ANN model results in some improvement in the standard deviation of temperatures compared to laminar chemistry as well.

The mean and $\text{rms}$ temperatures are compared for the third set of cases in Figures 5.70 and 5.71.
This set of cases included the LSM-MMD model and the LSM-SS-H model. Both models have mean temperatures that are only slightly cooler at the first station compared to laminar chemistry. The models also improve the mean temperatures at the second station as well, with temperatures that match more closely with the experiment. The LSM-SS-H model appears to match the experiment the closest at the third and fourth stations for the third set of cases. The LSM-MMD model results in cooler temperatures than laminar chemistry at all stations. It is again observed that the closure models result in smaller standard deviations in temperature compared to laminar chemistry.

Figure 5.66: Comparison of mean temperature for case set 1.
Figure 5.67: Comparison of $rms$ of temperature for case set 1.
Figure 5.68: Comparison of mean temperature for case set 2.
Figure 5.69: Comparison of $rms$ of temperature for case set 2.
Figure 5.70: Comparison of mean temperature for case set 3.
Figure 5.71: Comparison of $rms$ of temperature for case set 3.
Figure 5.72: Comparison of enhancement factor prediction for configuration C (same contour levels).
Figure 5.73: Comparison of enhancement factor prediction for configuration C (contours vary by station).
Figures 5.72 and 5.73 compare the time-averaged model enhancement factors for all the models tested for configuration C. The locations of large attenuation \((f < 1)\) correspond to locations where the mean temperature was decreased. The LSM-FS, LSM-FS-H, and JMP-ANN also predict some level of augmentation of reaction at some locations. The LSM-FS model results in some enhancement of reactivity on the bottom edge of the flame at the first station (as was observed for configuration A). The LSM-FS-H model also enhances reactivity in this region along with the entire outer edge of the flame at the second station. The JMP-ANN model appears to enhance reactivity within the jet of fuel, while attenuating in the developing flame near the top wall. The JMP-ANN and LSM-SS-H models result in much greater attenuation of reactivity at the first two stations compared to the other models. By the last station all models are essentially no longer active with mean values near one. It is important to note that all models appear to attenuate reactivity in similar regions of the flame; the main differences in the models are in the level of attenuation and the possibility of augmentation of reactivity.

![Enhancement Factor](image)

Figure 5.74: Centerplane average enhancement factor for models LSM-SS-H (top), LSM-MMD, LSM-JMPANN, LSM-FS-H, and LSM-FS (bottom).

Centerplane comparisons of the enhancement factors are shown in Figure 5.74. From top to bottom the models used are: LSM-SS-H, LSM-MMD, LSM-JMPANN, LSM-FS-H, and LSM-FS. The LSM-
Figure 5.75: Centerplane average temperature for models LSM-SS-H (top), LSM-MMD, LSM-JMPANN, LSM-FS-H, and LSM-FS (bottom).

JMPANN model attenuates the most in the ignition region, while the LSM-SS-H model attenuates over the largest region, followed by the LSM-MMD model. Centerplane contours of mean temperature are compared in Figure 5.75. It is clear that the locations of large amounts of augmentation predicted by the LSM-FS and LSM-FS-H models correspond to the cold region of high fuel concentration, which likely doesn’t have much effect on the averaged solution. The temperature contours are very similar between cases, with the LSM-JMPANN model results appearing to be the overall coolest.

Finally, instantaneous comparisons between model enhancement factors are shown in Figures 5.76 through 5.78. These figures show that the LSM-MMD and LSM-SS-H models result in more smooth contours compared to LSM-FS or LSM-FS-H. Allowing for augmentation of reactivity results in more discontinuous predictions of the enhancement factor as the models attempt to enhance reactivity across high-strain regions yet attenuate within areas of high-reactivity.
Figure 5.76: Instantaneous snapshots of enhancement factor for configuration C.

Figure 5.77: Instantaneous snapshots of enhancement factor for configuration C.
Figure 5.78: Instantaneous snapshots of enhancement factor for configuration C.
5.2.3 Configuration-E

A third test case was used to evaluate the effect of the LSM-FS model. This case corresponds to another experiment at UVa in which ethylene fuel was injected just upstream of a cavity flame holder. The cavity flame holder is fitted along the upper wall of the flow domain in order to increase the residence time and provide an ignition source for incoming fuel. There are options for injecting fuel at three different rows of injectors upstream of the cavity as well as a row of ports within the cavity, as shown in Figure 5.56; each row consists of five injectors. For the case presented here, ethylene is injected through the most upstream row of injectors at an equivalence ratio of $\phi = 0.15$. Other than replacement of the ramp injector with the cavity flame holder, the geometry is similar to configuration C. This case is also quite large, requiring a mesh with ~60M cells. The chemical mechanism for this simulation is the Taitech-Princeton (TP2) mechanism for ethylene combustion [53] which tracks 22 species. Previous results for this case were obtained using the laminar chemistry approach and are described in [39, 40].

For this work, this simulation was carried out for two CTTs to wash out any transient effects from implementing the LSM-FS model, with statistics taken for the following four CTTs. The simulations were initiated from a laminar chemistry solution from the previous study [39]. Figure 5.79 shows a centerline snapshot of temperature for this case; the location of the injector is indicated along with markers for the locations of which experimental data is available. The flame is anchored at the downstream edge of the cavity, and the flame appears to stay attached to the top wall without propagating far into the core of the tunnel. This lack of propagation is in stark contrast to the action of the hydrogen fueled cases which show the flame filling the flow domain; however the vertical extent of the flame does extend as it moves downstream. Analysis from [39] shows that this case is characterized by a rich, premixed flame near the cavity that transitions to a diffusion flame further downstream of the cavity.

For this case, simulation predictions using LSM-FS are compared with line-of-sight profiles extracted from TDLAS and WMS techniques [89, 91] along with results from a simulation using laminar chemistry [39] for three different stations. The first station is within the cavity at a location of $x/H = 2.38$, measured from the upstream edge of the cavity where $H$ is the depth of the cavity (~0.9 cm). The second and third stations are located downstream of the cavity at distances of $x/H = 6.56$ and 10.73, measured from the same location. Figures 5.80 - 5.82 compare water temperature, column density ($gm/m^2$), and mole fraction, respectively. Here it is observed that the mean temperatures have been decreased slightly as was observed in the previous cases. There are insignificant changes in water column density or mole fraction. Noticeable improvements are observed in the carbon monoxide temperature and column density as shown in Figures 5.83 and 5.84, respectively. Again, mean temperatures are lowered; more importantly, the column density of carbon monoxide is greatly reduced at the first station to match more closely with the experiment. Figure 5.85 shows carbon dioxide column density, which shows some slight improvement as well with the LSM-FS model being implemented.
Figure 5.79: Center-plane snapshot of temperature for configuration E.

Figure 5.80: $H_2O$ temperature for configuration E.

Figure 5.81: $H_2O$ column density for configuration E.
Figure 5.82: H$_2$O mole fraction for configuration E.

Figure 5.83: CO temperature for configuration E.

Figure 5.84: CO column density for configuration E.
Figure 5.85: CO$_2$ column density for configuration E.

Figure 5.86 shows the time-averaged enhancement factor at each of the three stations for configuration E. For this case, the average enhancement factor values vary between ~0.9 to 1.15 for all three stations. This indicates that the model is less active in this case compared to the previous hydrogen fueled cases. The model is biased towards augmentation of reactivity in the middle of the combustor, and attenuates near the cavity sidewalls. An analysis of the cavity flow (presented in [39]) shows two toroidal vortices are present within the cavity. The hotter, well-mixed regions within these vortex cores correspond to the location of attenuation while the high strain region between these vortices corresponds to the location at which the model enhances reactivity. This response is similar to the response of the model in configurations A and C, where the model also enhances reactivity along the high strain edges of the flame.

Figure 5.86: Mean enhancement factor for configuration E.
5.3 Volvo Bluff Body Case

An additional case was run to examine how the new family of models would perform for a low-speed, turbulent, premixed flame. This case corresponded to the Volvo Validation Rig; the geometry is shown in Figure 5.87. The domain consists of a top and bottom wall with a prism shaped bluff body flame-holder between the two. The case involves a mixture of propane and air entering at a fixed flow rate and temperature. The premixed gas passes over the bluff body which holds the flame by creating a recirculation zone of hot products. These hot products serve as the ignition source for the continual flow of reactants. The case simulated in this work used an inlet mass flow rate of 0.2 kg/s and an inflow temperature of 288.2 K. It should be noted that the experimental mass flow rate was three times larger due to the width of the combustor being three times larger than the computational domain. Experimental data from [92, 93] is available for comparison with the simulations. The experimental data includes profiles of static temperature, velocities, \(\text{rms}\) value of velocity fluctuations, and CO mass-fractions at various transverse stations. Centerline profiles for axial velocity and turbulence intensity is also available for comparison.

![Figure 5.87: Geometry for Volvo combustion rig.](image)

For this case, a two step, five species reaction mechanism for propane-air combustion was used [54]. This reaction mechanism is summarized in Appendix A.2. The REACTMB solver also required some modifications to handle the low speed flow. This required the use of the ‘all-speed’ LDFSS scheme [94] as well as a preconditioner [95] to update partial pressures rather than species densities. The Crank-Nicholson time-integration method was also replaced by a 3-point backward time discretization. Further, a new essentially non-oscillating PPM (ENO-PPM) scheme was implemented and used to generate all of the results reported in this section.

The results presented in this work were computed using a series of grids with isotropic grid resolutions of 1 mm, 2 mm, and 4 mm in the region of the flame. The grids consisted of approximately
10, 1.2, and 0.35 million cells for the fine, medium, and coarse grids, respectively. The topology of the mesh in the region of the flameholder is shown in Figure 5.88 for the medium-grid. The medium-grid was used for studying the effects of three different closure models. Since a third of the actual width of the combustor was considered in the simulation, periodic boundary conditions were used for the side plane boundary conditions. Fixed temperature and mass-flow rate boundary conditions were imposed at the inlet while a fixed back pressure of 100 kPa was used at the outlet. A fixed time step of $3.5 \times 10^{-6}$ seconds was used for the fine-mesh simulation, while $5.0 \times 10^{-6}$ seconds was used for the medium- and coarse-grid simulations. Instantaneous and time-averaged centerplane contours of temperature are compared in Figure 5.89 for the case of laminar chemistry on the 2 mm grid. Note the wrinkling of the flame front in the instantaneous snapshot. For this case, predictions using laminar chemistry, LSM-FS, LSM-MMD and LSM-Damk (Eq. 4.108) are compared with the experimental results. Temperature, velocity, $rms$ of velocity fluctuations, and turbulence intensities (defined by Eq. 5.3) are all compared for the stations available.

$$TI = \sqrt{U'_{rms}^2 + V'_{rms}^2}$$

(5.3)

![Figure 5.88: Mesh topology for 2mm grid resolution near the flameholder.](image)

### 5.3.1 Modeling Study

Figure 5.90 compares the mean temperatures for each simulation versus the experimental data for the 2 mm mesh resolution. All simulations result in over-prediction of peak temperatures by the last station while predicting less spreading of the flame compared to the experiment. However, the LSM based closure models appear to attenuate the temperature to a small degree at all stations matching more closely with the experiment, especially at the first station.
Figures 5.91 and 5.93 compare mean axial velocity for axial and transverse profiles, respectively. These show that using any of the LSM closures results in a better matching between the extent of the recirculation zones predicted by the simulations and the experiment. Further downstream, the simulation using laminar chemistry is exiting the domain faster, while the LSM-FS model shows mean velocity profiles that match the experiment the closest. Figure 5.94 compares transverse velocity profiles for each case, which show less variation. It appears that implementing the LSM based models damps some of the peaks in the transverse velocity profiles. Note that all quantities are normalized by the bulk velocity (17.3 m/s).

Figures 5.95 and 5.96 compare the standard deviations of the axial and transverse velocity components. In figure 5.95, some decrease in the peak values are observed when the LSM based models are implemented. For the case of the transverse velocity, there is a large change in the $rms$ profiles when any of the LSM based models are implemented compared to laminar chemistry, matching much more closely with the experiment. Figure 5.92 compares the 2D turbulence intensity, as defined by Eq. 5.3, between cases. As expected, from the shifts in velocity fluctuations, the turbulence intensities drop upon
implementing any of the LSM based models. The LSM-MMD and LSM-Damk models are somewhat closer to the experiment relative to LSM-FS and laminar chemistry. The observed decrease in turbulence intensity is likely related to the action of the models in filtering species production rates, thus reducing the intensity of heat release and local flame speeds.

From the results discussed, the LSM models presented all perform very similarly to one another. Further distinction of the model effects can be seen by comparing average enhancement factors for each model. Figure 5.97 compares centerplane contours of the average enhancement factors for each model. Note that the LSM-MMD model attenuates the most at the flameholder edges followed by LSM-Damk and LSM-FS. This figure also highlights an issue with visualizing the enhancement factor for premixed flames that allow for attenuation. The LSM-FS model contour plot shows a large amount of enhancement although the flame temperatures and heat release actually drop. This is because enhancement is being predicted for locations surrounding the flame that have production rates near zero.

### 5.3.2 Mesh Refinement Study

A mesh refinement study was also carried out for this case. The grid resolutions considered corresponded to isotropic mesh widths of 1 mm, 2 mm, and 4 mm in the region of the flame for the fine, medium and coarse grids, respectively. Figure 5.98 compares snapshots from for each of these grid resolutions. Comparisons are made between temperature, vorticity and enhancement factor. Note that the vorticity plot shows an increase in the number of resolved eddy structures as would be expected with mesh refinement. Also, a thinning of the flame front in both the temperature and enhancement factor contours.
is observed. The response of the enhancement factor is similar to thickened flame models in that it is confined to the flame front. Enhancement factor values appear to be approximately 0.75 through much of the flame front.

Figures 5.99 through 5.105 compare the temperature, turbulence intensity and velocity profiles for different grid resolutions for the case with LSM-MMD and the ENO-PPM scheme. Mean temperature profiles are compared in Figure 5.99; the trends here show that refining the grid results in a broadening of the flame as well as some decrease in peak flame temperature. This is due to increased vortex shedding with grid refinement. This motion results in pulling of pockets of colder fluid into the centerline and spreading of the hot reacting gases outward. This can be observed in the temperature snapshots in Figure 5.98.

Figures 5.100 and 5.102 compare mean axial profiles. These figures show general improvement in experimental data agreement with mesh refinement. Figure 5.103 compares mean transverse velocity profiles which are less sensitive to grid refinement. The coarsest mesh has noticeably sharper peaks in the axial velocity profiles at the centerline of the domain. The medium and fine grid results are very similar, with grid refinement improving the profiles towards the exit of the domain.

Figure 5.101 compares turbulence intensity with grid refinement. The increased resolution helps to capture the appropriate turbulence intensity growth from the back wall of the flameholder, within the recirculation zone. Figures 5.104 and 5.105 compare velocity fluctuations. For both axial and transverse velocity fluctuations, the peaks are reduced with increased grid resolution to match more closely with the experiment. This is consistent with the capturing of the smaller-scale eddy structures, which results in less intense fluctuations.

5.3.3 Lean Blowout Simulations

Finally, simulations were conducted to study the lean blowout limit of the Volvo combustor. All models were implemented for a case with an equivalence ratio of 0.55; the simulations were initiated from a solution with the previous equivalence ratio of 0.65. The composition change was enforced at the inlet plane. Figure 5.106 shows the total volumetric heat release over time for each of the models implemented, including laminar chemistry as well as heat release variation with grid refinement. Clearly, the flame blows out for the LSM-MMD and LSM-FS models in approximately the same amount of time. Meanwhile, neither the laminar chemistry or LSM-Damk cases blow off. The LSM-Damk model likely doesn’t result in flame blowout due to the blending with laminar chemistry near the flameholder which results in enhancement factor values closer to one. All cases with the LSM-MMD model, for varying grid resolution, eventually blowout. The coarsest grid blows out the quickest while the medium and fine grids blowout in roughly the same time. Note that this figure does not indicate the time at which the flame disconnects from the back of the flameholder as global heat release will only diminishes when
flame elements exit the domain without being replenished.

Figure 5.107 compares snapshots of temperature contours for the transition to the lower equivalence ratio corresponding to the lean blowout conditions on the 2 mm grid. Although a drop in temperature and heat release is observed when laminar chemistry is used, the flame does not blowout. The LSM-MMD transition is also shown in Figure 5.107. The LSM-MMD model resulted in attenuation of reactivity along the flame front relative to laminar chemistry. This, combined with the lower equivalence ratio, resulted in a drop in the turbulent flame speed but an increase in wrinkling and flame surface area. This causes increased turbulent intensity as well as asymmetric vortex shedding which eventually shrinks the recirculation zone until the flame detaches. Once the flame is disconnected from the recirculation zone, the remaining reactive pockets will eventually translate out of the domain.
Figure 5.92: Comparison of centerline turbulence intensity profiles.

Figure 5.93: Comparison of mean axial velocity velocity.
Figure 5.94: Comparison of mean transverse velocity.
Figure 5.95: Comparison of \textit{rms} of axial velocity fluctuations.
Figure 5.96: Comparison of $rms$ of transverse velocity fluctuations.
Figure 5.97: Average enhancement factor values for Volvo case.
Figure 5.98: Comparisons of vorticity (top), temperature (bottom left) and enhancement factor (bottom right) with changing grid resolution: fine (top), medium (middle) and coarse (bottom).

Figure 5.99: Comparison of mean temperature with grid refinement.
Figure 5.100: Comparison of centerline mean axial velocity with grid refinement.

Figure 5.101: Comparison of centerline turbulence intensity profiles with grid refinement.
Figure 5.102: Comparison of mean axial velocity with grid refinement.
Figure 5.103: Comparison of mean transverse velocity with grid refinement.
Figure 5.104: Comparison of \( \text{rms} \) of axial velocity fluctuations with grid refinement.
Figure 5.105: Comparison of $rms$ of transverse velocity fluctuations with grid refinement.
Figure 5.106: Heat release time history for lean blowout case.

Figure 5.107: Evolution of temperature contours during transition to lower equivalence with laminar chemistry (left) and LSM-MMD (right).
Chapter 6

Conclusions and Future Work

The work performed in this study focused on the definition, assessment, and testing of a new family of chemical closure models for high-speed LES. The goal was to develop models that could easily be implemented into a Eulerian based solver that utilizes finite-rate chemistry. Finite-rate chemistry is the method of choice due to the complex nature of high speed reacting flows which involve compressibility effects, shock/plume interactions, transient events and short convective time scales. The downside to using finite-rate chemistry is that individual species must be transported, and their filtered chemical production rates calculated. Typical reaction mechanisms can involve dozens of species and hundreds of reactions; therefore, evaluating the filtered chemical production rates using laminar chemistry is already somewhat expensive. To reduce any additional costs, relatively inexpensive models were desired to account for the effects of unresolved turbulence on apparent reactivity at a given mesh scale. A new family of closure models was developed guided by the use of mesh-sequenced realizations. These models were developed from a least-squares minimization between filtered fine-grid chemical source terms and the resolved chemical source terms using laminar chemistry, for a given grid level.

A mesh-sequenced realization / modified a priori analysis framework was described and was used to develop various closures that account for the turbulent fluctuations resolved via grid refinement. This analysis used an idealized combustion chamber that was evolved, simultaneously on a fine and coarse grid. The coarse grid was constrained by the fine-mesh velocity field in order to ensure that the eddy evolution between grid levels was highly correlated so that discrete points in space and time could be compared. Flow data was extracted from a number of discrete locations, and used to analyze the difference in chemical production rates between grid levels due to unresolved turbulent fluctuations on the coarse-grid compared to the fine. The baseline model developed was the LSM-FS model, or least-squares minimization-filtered sources model. This model applies a test filter to the chemical source terms in the nearest 27 cells to close the model. Heat release can also be implemented into the model to obtain the LSM-FS with heat (or LSM-FS-H) model. Another variation is the LSM-MMD model
which applies a min-mod operator to ensure that the minimum between the test filtered and laminar chemistry predicted source term is used. A scale-similarity closure model was also defined and tested. Finally, models built around correlated an ‘optimal single point’ in the neighborhood of cells were also investigated.

After initial tests, select models were further evaluated for cases for which experimental data was available. Three of these cases corresponded to experiments conducted at the University of Virginia (UVa). The final case investigated was a low speed, turbulent premixed flame corresponding to the Volvo Validation Rig. The LSM-FS model was tested for each of these cases. Other LSM variants were tested for configuration C combustor and the Volvo experiment. In the hydrogen-fueled configurations A and C combustors, the model enhanced reactivity in the ignition region, along the lower side of the developing flame. The model attenuates reactivity in the low momentum region on the top side of the flow domain and further downstream where the flame has propagated into the center of the domain. In the ethylene-fueled configuration E combustor, the model attenuated reactivity within the toroidal vortices and enhanced reactivity in the high strain region between these vortices. The model was much less active in this case; it is not clear if this was due to grid resolution, the chemical kinetics, or turbulence levels. These observations lead to the conclusion that the LSM-FS model tends to attenuate reactivity in well mixed, highly reactive regions and augment reactivity in high strain regions.

Configuration C served as the test case for comparing several models including: LSM-FS, LSM-FS-H, LSM-JMPANN, LSM-MMD, and LSM-SS-H. Comparing LSM-FS and LSM-FS-H results led to the conclusion that incorporating heat release into the model results in more augmentation of reactivity in the high-strain regions. All models attenuated in regions of well mixed, highly reactive flamelets, and resulted in lower fluctuations in flow variables, due to the filtering operations. The LSM-JMPANN and LSM-SS-H models resulted in the coolest peak temperatures at the first stations of configuration C, matching the best with the experiment. Agreement with experimental data at the remaining stations was generally improved by the application of any of the models. From these comparisons it is concluded that the level of attenuation predicted by the LSM based closure models is likely more important than augmentation.

The final case considered was the propane-fueled Volvo Validation Rig. This case is different in that it is both low-speed and premixed. The LSM-FS, LSM-MMD, and LSM-Damk models were tested for this case. Similar to other cases, all closure models decreased temperature relative to the laminar chemistry model. Since this was a premixed flame, some additional observations were made. Due to the filtering operation, the model results in some smoothing of the flame and thus a reduction in heat release and local flame speed can be expected. This was reflected in the results where reductions in velocity fluctuations, turbulence intensity, and heat release were observed relative to laminar chemistry; these trends were consistent with experimental results as well. The case was also tested at lean blowout conditions. The LSM-FS and LSM-MMD models were able to predict flame blowout, while the simulation
with laminar chemistry would not blowout. The primary conclusion drawn from these results is that the LSM type models results in action similar to that of thickened flame models for premixed flames, where the reactivity is attenuated along the flame front by a roughly constant value of approximately 0.75.

In conclusion, a new family of simple closure models for the filtered chemical production rates have been derived. These models require a small amount of additional computational work, relative to laminar chemistry, and provide a modest, yet consistent, improvement in predictive capability. Taking into consideration cost and overall complexity in implementation, the LSM-FS model is still the overall preferred model with the LSM-MMD model being a close second. The LSM-FS model is preferred simply due to its ability to enhance reactivity and the lack of definitive evidence that turbulent fluctuations always result in less reactivity compared to that predicted by laminar chemistry. Further, results indicate that correlations exist between quantifiable flow variables (e.g. Damköhler number, mixture fraction, or $R_M$) and the exact LSM enhancement factor, and that these can be exploited to provide extensions to the model formulation.

This work has opened up various areas for future work. First and foremost, there is still a need for understanding the coupled effects of grid resolution, numerics, and choice of closure model for turbulent reactive flow simulations. Second, there is certainly room for extension of the models proposed in this work to incorporate other information. Grid spacing and Damköhler number are two quantities that have recently been considered; however, more work is needed to determine how the information can be used. Third, the ‘optimal single point’ models implemented in this work showed some promise, and could provide for another area for future investigation. One idea that has not yet been investigated is the potential for machine learning to model the $R_M$ values discussed in Section 4.10.6. The definition for $R_M$ is ideal for neural networks as it is normalized between 0 and 1 for every cell, and could potentially be modeled as a function of other reduced variables, such as mixture fraction, or progress variables. Finally, further investigation into the effect of these closure models on premixed flames is warranted. Since the modified a priori analysis was conducted for a supersonic, non-premixed flame, it is not clear if some of the conclusions drawn, such as the optimal filter width, hold true for a premixed flame.
REFERENCES


Appendix A

Reaction Mechanisms
A.1 Burke Mechanism

This section details the Burke hydrogen-air mechanism used in this work. The units for this mechanism are seconds, moles, centimeters, calories, and degrees Kelvin. The units of the activation energy $E_A$ are cal mol$^{-1}$ K$^{-1}$. The units of the pre-exponential factor, $A$, is determined for each reaction from dimensional analysis. Third-body efficiencies and Troe efficiencies are also tabulated.

Table A.1: Burke mechanism.

<table>
<thead>
<tr>
<th>Rxn No.</th>
<th>Reaction</th>
<th>$A$</th>
<th>$\eta$</th>
<th>$E_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H + O_2 \Leftrightarrow O + OH$</td>
<td>$1.04 \times 10^{14}$</td>
<td>0.0</td>
<td>$1.531 \times 10^{4}$</td>
</tr>
<tr>
<td>2</td>
<td>$O + H_2 \Leftrightarrow H + OH$</td>
<td>dup. $3.82 \times 10^{12}$</td>
<td>0.0</td>
<td>$7.948 \times 10^{3}$</td>
</tr>
<tr>
<td></td>
<td>dup.</td>
<td>dup. $8.79 \times 10^{14}$</td>
<td>0.0</td>
<td>$1.917 \times 10^{4}$</td>
</tr>
<tr>
<td>3</td>
<td>$H_2 + OH \Leftrightarrow H_2O + H$</td>
<td>$2.16 \times 10^{8}$</td>
<td>1.51</td>
<td>$3.430 \times 10^{3}$</td>
</tr>
<tr>
<td>4</td>
<td>$OH + OH \Leftrightarrow O + H_2O$</td>
<td>$3.34 \times 10^{4}$</td>
<td>2.42</td>
<td>$-1.930 \times 10^{3}$</td>
</tr>
<tr>
<td>5</td>
<td>$H_2 + M \Leftrightarrow H + H + M$</td>
<td>$4.58 \times 10^{10}$</td>
<td>-1.40</td>
<td>$1.040 \times 10^{5}$</td>
</tr>
<tr>
<td>6</td>
<td>$O + O + M \Leftrightarrow O_2 + M$</td>
<td>$6.16 \times 10^{15}$</td>
<td>-0.50</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>$O + H + M \Leftrightarrow OH + M$</td>
<td>$4.17 \times 10^{18}$</td>
<td>-1.00</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>$H_2O + M \Leftrightarrow H + OH + M$</td>
<td>$6.06 \times 10^{27}$</td>
<td>-3.32</td>
<td>$1.208 \times 10^{5}$</td>
</tr>
<tr>
<td>9</td>
<td>$H + O_2 + M \Leftrightarrow HO_2 + M$</td>
<td>$6.37 \times 10^{20}$</td>
<td>-1.72</td>
<td>$5.250 \times 10^{2}$</td>
</tr>
<tr>
<td></td>
<td>dup.</td>
<td>$k_{f,0}$ $4.65 \times 10^{12}$</td>
<td>0.44</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>$HO_2 + H \Leftrightarrow H_2O + O_2$</td>
<td>$2.75 \times 10^{6}$</td>
<td>2.09</td>
<td>$-1.451 \times 10^{3}$</td>
</tr>
<tr>
<td>11</td>
<td>$HO_2 + H \Leftrightarrow OH + OH$</td>
<td>$7.08 \times 10^{13}$</td>
<td>0.0</td>
<td>$2.950 \times 10^{2}$</td>
</tr>
<tr>
<td>12</td>
<td>$HO_2 + O \Leftrightarrow O_2 + OH$</td>
<td>$2.85 \times 10^{10}$</td>
<td>1.00</td>
<td>$-7.239 \times 10^{2}$</td>
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<tr>
<td>13</td>
<td>$HO_2 + OH \Leftrightarrow H_2O + O_2$</td>
<td>$2.89 \times 10^{13}$</td>
<td>0.0</td>
<td>$-4.970 \times 10^{2}$</td>
</tr>
<tr>
<td>14</td>
<td>$HO_2 + HO_2 \Leftrightarrow H_2O_2 + O_2$</td>
<td>dup. $4.20 \times 10^{14}$</td>
<td>0.0</td>
<td>$1.200 \times 10^{4}$</td>
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<tr>
<td></td>
<td>dup.</td>
<td>$k_{f,0}$ $1.30 \times 10^{11}$</td>
<td>0.0</td>
<td>$-1.630 \times 10^{3}$</td>
</tr>
<tr>
<td>15</td>
<td>$H_2O_2 + M \Leftrightarrow OH + OH + M$</td>
<td>dup. $2.49 \times 10^{24}$</td>
<td>-2.30</td>
<td>$4.875 \times 10^{4}$</td>
</tr>
<tr>
<td></td>
<td>dup.</td>
<td>$k_{f,0}$ $2.00 \times 10^{12}$</td>
<td>0.90</td>
<td>$4.875 \times 10^{4}$</td>
</tr>
<tr>
<td>16</td>
<td>$H_2O_2 + H \Leftrightarrow H_2O + OH$</td>
<td>$2.41 \times 10^{13}$</td>
<td>0.0</td>
<td>$3.970 \times 10^{3}$</td>
</tr>
<tr>
<td>17</td>
<td>$H_2O_2 + H \Leftrightarrow HO_2 + H_2$</td>
<td>$4.82 \times 10^{13}$</td>
<td>0.0</td>
<td>$7.950 \times 10^{3}$</td>
</tr>
<tr>
<td>18</td>
<td>$H_2O_2 + O \Leftrightarrow OH + H_2O$</td>
<td>$9.55 \times 10^{9}$</td>
<td>2.00</td>
<td>$3.970 \times 10^{3}$</td>
</tr>
<tr>
<td>19</td>
<td>$H_2O_2 + OH \Leftrightarrow HO_2 + H_2O$</td>
<td>dup. $1.74 \times 10^{12}$</td>
<td>0.0</td>
<td>$3.180 \times 10^{2}$</td>
</tr>
<tr>
<td></td>
<td>dup.</td>
<td>dup. $7.59 \times 10^{13}$</td>
<td>0.0</td>
<td>$7.270 \times 10^{3}$</td>
</tr>
</tbody>
</table>
Table A.2: Chaperon efficiencies for third-body dissociation reactions in the Burke mechanism.

<table>
<thead>
<tr>
<th></th>
<th>N₂</th>
<th>O₂</th>
<th>H₂</th>
<th>H₂O</th>
<th>H₂O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>R5</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
</tr>
<tr>
<td>R6</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
</tr>
<tr>
<td>R7</td>
<td>1.0</td>
<td>1.0</td>
<td>2.5</td>
<td>12.0</td>
<td>1.0</td>
</tr>
<tr>
<td>R8</td>
<td>2.0</td>
<td>1.5</td>
<td>3.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>R9a</td>
<td>1.0</td>
<td>0.78</td>
<td>2.0</td>
<td>14.0</td>
<td>1.0</td>
</tr>
<tr>
<td>R15a</td>
<td>1.5</td>
<td>1.2</td>
<td>3.7</td>
<td>7.5</td>
<td>7.7</td>
</tr>
</tbody>
</table>

Table A.3: Troe coefficients for Burke mechanism.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>T*</th>
<th>T**</th>
<th>T***</th>
</tr>
</thead>
<tbody>
<tr>
<td>R9</td>
<td>0.5</td>
<td>1.0 × 10³⁰</td>
<td>0.0</td>
<td>1.0 × 10⁻³⁰</td>
</tr>
<tr>
<td>R15</td>
<td>0.42</td>
<td>1.0 × 10³⁰</td>
<td>0.0</td>
<td>1.0 × 10⁻³⁰</td>
</tr>
</tbody>
</table>

A.2 Propane-Air 2-step Mechanism

The two-step propane-air reaction mechanism is summarized by the following equations. Here $q_1$ and $q_2$ are the net rate of reactions. Note that reaction one is forward only. The constants are summarized in Table A.4. For this mechanism the pre-exponential factors have units of centimeters, grams, and seconds. The activation energy has units of cal mol⁻¹.

\[ C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O \]
\[ CO + 0.5O_2 \rightleftharpoons CO_2 \]  \hspace{1cm} (A.1)

\[ q_1 = A_1 \left( \frac{\rho_{C_3H_8}}{\rho_{O_2}} \right)^{0.9028} \left( \frac{\rho_{O_2}}{\rho_{CO}} \right)^{0.6855} \exp \left( \frac{-E_1}{RT} \right) \]

\[ q_2 = A_2 \left[ \left( \frac{\rho_{CO}}{\rho_{O_2}} \right)^{1.0} \left( \frac{\rho_{O_2}}{\rho_{CO_2}} \right)^{0.5} - \frac{1}{K_{eq}} \left( \frac{\rho_{CO_2}}{\rho_{CO}} \right)^{1.0} \right] \exp \left( \frac{-E_2}{RT} \right) \]  \hspace{1cm} (A.2)

Table A.4: Propane-Air reaction coefficients.

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>2.0 × 10¹²</td>
<td>3.3 × 10⁴</td>
</tr>
<tr>
<td>R2</td>
<td>4.5 × 10¹⁰</td>
<td>1.2 × 10⁴</td>
</tr>
</tbody>
</table>
A.3 Taitech/Princeton Mechanism (TP-2)

Ethylene combustion was modeled using the Taitech/Princeton reduced ethylene kinetics model, TP-2 [53], which consists of 22-species. This mechanism is available as a Fortran subroutine, which requires pressure, temperature and species mass-fractions as inputs and outputs the species production rates. In the version of REACTMB used to conduct the ethylene fueled configuration, the species production rates and their Jacobians are calculated using this routine. Jacobians are calculated by calling the Fortran routine repeatedly with small perturbations in the input quantity for which derivatives are being estimated. This increases the cost associated with using this mechanism. The sum of the production rates of all species, as calculated by the routine, is not identically zero. Eq. A.3 is used to enforce the condition that the sum of the species production rates is zero.

\[
\dot{\omega}_s = \dot{\omega}_s^{TP2} - \sum_{i=1}^{NS} Y_i \dot{\omega}_i^{TP2}
\]  

(A.3)
Appendix B

Additional Config. C Results
B.1 Additional Comparisons for Configuration C

Figure B.1: Comparison of mean nitrogen mole fraction for case set 1.
Figure B.2: Comparison of $rms$ of nitrogen mole fraction for case set 1.
Figure B.3: Comparison of mean oxygen mole fraction for case set 1.
Figure B.4: Comparison of rms of oxygen mole fraction for case set 1.
Figure B.5: Comparison of mean hydrogen mole fraction for case set 1.
Figure B.6: Comparison of $rms$ of hydrogen mole fraction for case set 1.
Figure B.7: Comparison of mean nitrogen mole fraction for case set 2.
Figure B.8: Comparison of $rms$ of nitrogen mole fraction for case set 2.
Figure B.9: Comparison of mean oxygen mole fraction for case set 2.
Figure B.10: Comparison of $rms$ of oxygen mole fraction for case set 2.
Figure B.11: Comparison of mean hydrogen mole fraction for case set 2.
Figure B.12: Comparison of $rms$ of hydrogen mole fraction for case set 2.
Figure B.13: Comparison of mean nitrogen mole fraction for case set 3.
Figure B.14: Comparison of rms of nitrogen mole fraction for case set 3.
Figure B.15: Comparison of mean oxygen mole fraction for case set 3.
Figure B.16: Comparison of \textit{rms} of oxygen mole fraction for case set 3.
Figure B.17: Comparison of mean hydrogen mole fraction for case set 3.
Figure B.18: Comparison of \( \text{rms} \) of hydrogen mole fraction for case set 3.