ABSTRACT

MILES, JEFFERY SCOTT. ODT Based Closure Model for Non-Premixed Combustion LES. (Under the direction of Dr. Tarek Echekki).

An LES closure method for turbulent non-premixed combustion using data from stand-alone ODT simulations is developed and validated. An ODT simulation provides a complete view of turbulent combustion including detailed chemistry within a single dimension through spatially (in 1D) and temporally resolved solutions for thermo chemical scalars and a stochastic description of turbulent advection. A unique closure technique removes the limitations associated with prescribed FDF distributions by using the resolved ODT statistics to construct joint scalar distributions needed for LES closure. These distributions are combined with other ODT statistics to construct closure tables for filtered variables such as density and chemical source terms. The tabulated closure follows the classical integration over state-space combining joint distributions with statistics from dependent variables. The temperature and mixture fraction are considered for this joint FDF as they can be combined to provide a complete view of the chemical and thermal state of the overall system within a non-premixed combustion problem. The ODT simulations are used to extract filtered and unfiltered correlations representing FDF distributions for each of the state-defining scalars; and kernel density functions are used to convert the sample datasets into smooth distributions that represent FDFs found within ODT statistics.

A stand-alone ODT simulation is configured to generate the statistics and data needed for the closure model construction. The ODT domain selected to match the target problem domain is a one-dimensional axisymmetric piloted jet. This configuration is capable of capturing many of the features of a turbulent jet diffusion flame much like a spatially resolved DNS simulation but at a fraction of the cost. For each realization, the state variables are filtered
and stored in vector form with the “instantaneous” values for each term included in the un-closed set required in the LES domain. Model construction as well as the methods applied for data processing are described in addition to the design and application of LES closure. OpenFOAM, an open-source extensible CFD package, is used to implement the LES simulation needed to verify the proposed closure model.

The LES-ODT closure model is validated using the Sandia Flame (D & F) family of piloted jet diffusion flames, which are excellent test cases to demonstrate the effects of turbulence in non-premixed combustion. The LES-ODT closure model exhibits good correlation with experimental results while also reproducing salient features associated with these flames, including the occurrence of extinction and re-ignition. Evidence of such occurrences is analyzed within the LES domain through comparisons of conditional statistics of species mass fractions as well as spatial contour plots of temperature, species mass fractions and scalar dissipation. The results of these comparisons demonstrate the capacity for the LES-ODT closure model to capture the interactions between turbulence and chemistry within non-premixed combustion problems. Other features such as entrainment and scalar mixing are also investigated through axial and radial profiles extracted from the LES results.
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ODT Based Closure Model for Non-Premixed Combustion 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

Mechanical Engineering

Raleigh, North Carolina

2017

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DEDICATION

I dedicate this dissertation to Twila, my wife of 25 years. She is the love of my life and continues to fill my heart with joy every day. Through all of my many pursuits, she continues to stand by me and support my decisions. She is sad when we fail, and she is happy when we succeed. But she is always by my side, continuing in her faithfulness. She is the heart of our family and she continues to amaze with her encouraging words. Through this experience our relationship has been made stronger, making my hope for the future bright. As we press on, I pray that our lives will forever be blessed with the joy and hope that comes with love.
BIOGRAPHY

Jeffery Miles was born in Wooster, Ohio in 1970, but at a very young age, he moved south to North Carolina with his parents. After many different relocations and changes of address, Jeffery finally settled in Hickory, NC with his parents and 4 of his siblings. Jeffery gained a strong interest in computers at a very young age, and after high school chose to attend NC State, studying Computer Engineering. Even though Jeffery’s interest in computers centered more around the physics of the hardware, after graduation, he choose to pursue a career in software development. At the same time Jeffery was married to Twila whom he had met years before. Being newly married and working in software development, Jeffery and Twila set out to live a normal suburban lifestyle.

After working for more than 10 years in software development, Jeffery decided to try something different. With the help of two of his brothers, Jeffery built and raced a late-model stock car. Unfortunately, with the financials of the operation falling short, the racing business and his racing career came to an end, sooner than expected. All throughout the experience, Jeffery realized that science behind the race car was more interesting than the race car itself. Thus, after exiting his short racing career, Jeffery explored academic opportunities that align with automotive technologies. In the spring of 2005 Jeffery started a Master’s degree in mechanical engineering at NC State. After taking a few classes, combustion surfaced as a topic that interested Jeffery most. It was this interest combined with his remaining interest in computers that enticed him to purse a PhD in mechanical engineering focused on computation and combustion.

Jeffery and Twila have now been married for 25 years, and they have five children. Madison is 12 years old and in the 6th grade. Felicia is 13 years old and in the 8th grade. Jeffery
is 16 years old and in the 11th grade. Abigail is 17 years old in the 12th grade. And Carl is 18 years old in the 11th grade. Carl was the last addition to the family in that he was adopted from an orphanage in Ukraine. Carl came the US in 2010 and has been a blessing ever since.
ACKNOWLEDGMENTS

I would like to thank my wife and kids for their many years of sacrifice and support during my academic pursuits. Each in their own way has provided encouragement and motivation for me to continue through all these years. I would also like to thank my mother, Dr. Gail Miles, and my father, Vern Miles for their wisdom and guidance both in my education and in my life. Thanks, also, to my brother Dr. Jeremy Miles who continues to motivate me by demonstrating what is possible, and to my other siblings for their companionship and encouragement.

A special thanks goes out to Dr. Tarek Echekki for the many years of advice and support. This effort would not have been possible without his dedication and patience helping me to advance every step of the way. I would also like to thank Dr. Hong Luo, Dr. Jack Edwards and Dr. Kevin Lyons for their willingness to serve on my committee. They have all been very encouraging and helpful in every aspect of my research. A particular thanks, also, goes to Dr. Phil Westmoreland who agreed on a very short notice to serve on my committee. His enthusiasm is contagious, and I appreciate his many efforts to make NC State University a good experience for all the students and faculty that he encounters.

Finally, I am grateful for the many managers at Toshiba Global Commerce who I have had the privilege of working with all these years. They have given me the freedom and flexibility to pursue my education in a business climate that is less than favorable. A particular thanks goes to John Gatto, who encouraged and defended me the most at the beginning. His kind words and understanding helped me to see what I could accomplish.
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1 Introduction

1.1 Background and Motivation

Never before has the study of power generation and heating systems fueled by combustion of fossil fuels and bio-fuels been more important. Due to the never-ending threat of global warming and competition from alternative energy sources, efficiency and environmental conservation continue to grow as important factors in designing and applying these systems. A complementary concept that many times enhances the combustion process is turbulence. Making the overall system more efficient and effective, turbulence provides a mechanism by which available kinetic energy is leveraged in the mixing process. Unfortunately, this increased efficiency always comes with a price. Adding turbulence to a reacting flow enhances mixing, but it also increases the complexity and instability. Turbulence tends to affect the reaction mechanism just as system changes due to combustion affect the turbulent flow characteristics. The inability to capture this relationship completely can lead to inefficient system designs that generate more pollutants or waste more fuel. Modern research on the subject of turbulent combustion continues to focus on the interactions between turbulence and reacting flows to understand and leverage the benefits better while avoiding the pitfalls.

Recent engineering processes tend to rely heavily on computational simulations to evaluate system design choices. While computing power and numerical operations do incur a cost, the expense is much smaller compared to the overhead of building and analyzing design prototypes. When considering the time necessary to set up experiments as well as the scientific equipment needed to gather key data, the cost of traditional analysis is far greater than that of
setting up and running computer models. Experimental studies are necessary to understand the science governing a model, but long term results are best obtained from re-application of computer simulations which can be adjusted to fit requirements specific to a given domain. In general, there is an inverse relation between the degree of empiricism included in a model and the versatility of its application. Simulations that contain a higher degree of empiricism tend to work best for environments and domains which match that of the original design. Models that are more true to the physics while accounting for the numerical limits have a wider scope of application. Unfortunately, the complexity of turbulent combustions makes the balance between versatility and empiricism even more important. As a result, numerical studies which focus on turbulent combustion continue to be important and draw much attention within the energy research community.

At the core of any turbulent system is a series of fluid motions transferring energy downward from the largest length scales to the smallest. Energy provided in the bulk large scale motion is then dissipated within the smallest scales of the domain. Additionally, these smaller regions host molecular processes, such as diffusion and combustion, making for an even more complex small-scale problem. While much of what is visible occurs in the large scale portions of the domain, the truly interesting portion of the solution lies within the molecular scales. When the larger scales in a domain differ in size from the smallest scales by several orders of magnitude, the complexity of any numerical study must increase in order to accomplish acceptable accuracy. Furthermore, combustion within a turbulent flow field includes processes such as chemical reactions, thermal transfer and molecular mixing which are subject to different time scales. Each timescale can vary significantly, much like the length scales. Large differences in time scales add to the complexity of a numerical study. The
challenge then for any computer model is to capture the necessary time scales as well as the important length scales simultaneously using a reasonable amount of resources while also staying within a reasonable degree of accuracy.

1.2 Direct Numerical Simulation (DNS)

To be effective, a numerical solution designed to operate with a computer must solve the given problem efficiently while also containing the discretization and numerical errors. Due to the large differences in spatial and temporal scales mentioned above, a discrete solution which solves the differential equations governing a turbulent reacting system directly must operate within an extremely fine grid capable of capturing all the length scales. In addition, extremely small time steps may be required to capture all the time scales that are present. Direct solutions to the widely accepted Navier-Stokes equations governing a turbulent fluid flows are generally named Direct Numerical Solutions (DNS) due to the lack of simplifying models or assumptions. These solutions are strapped with scale and complexity limitations due to the many factors mentioned above. As discussed in (Veynante & Poinsot, 2005), the number of grid points needed to represent a turbulent flow problem properly at a given Reynolds number limit is proportional to the ratio of the largest scales to the smallest scales: 

\[
\frac{l}{\eta} < N
\]

A good domain definition must then balance the limitations on the size of the domain, limitations to the Reynolds number and limitations on the number of grid points.

\[
Re_t < N^{4/3}
\]  

(1.1)

When the flow includes chemical reactions, the ratio between the residence time and the chemical process (Damköhler number) plays a role further limiting the solution. Analysis
of reacting flows reveal that the grid must be small enough to capture the reaction mechanism within a given residence time, meaning the inner portion of the domain must be fine enough to resolve all of the flame elements represented in the regions surrounding a flame. As a result, limitations for a numerical simulation of a turbulent reacting flow can be expressed as the ratio of the largest scale in the domain to the flame thickness in conjunction with the ratio of the overall number of grid points and the inner region size needed to capture the flame. With $Q$ representing the number of grid points necessary to capture the important parts of a flame structure, this limitation relates the product of the turbulent Reynolds number and the Damköhler number to the square of inner and outer portions of the grid (Veynante & Poinset, 2005).

$$Re_tD_a < \left(\frac{N}{Q}\right)^2$$

(1.2)

The term $Re_tD_a$ is an expression which captures the combination of fluid motion and the speed of the small-scale processes. $\frac{N}{Q}$ is an expression which illustrates the cost of simultaneously capturing the large regions of the domain while also representing the physics occurring in the smaller portions. Eq. (1.2) explains the limitations of what DNS studies can accomplish with the allotted computational resources.

While research efforts continue to strive to improve the methods by which the Navier-Stokes equations are discretized, other active areas of research include innovative means to represent complex combustion mechanisms, as well as strategies to manage grid manipulation, to achieve more efficient results. When detailed chemistry is desirable, the computational overhead is a limiting factor in how much detail can be included. Even a simple five-step reaction mechanism adds hundreds of additional calculations for each grid point during a single
iteration of a computation. This complexity is generally not feasible for domains of any significant size. Intrinsic Low Dimensional Manifold (IDLM) is used to reduce the overall picture of a more detailed mechanism. This procedure separates the reactive species, focusing on the ones with slower chemical-reaction time scales. Requiring fewer species to reach a solution facilitates a more tractable solution, however, neglecting the species with faster time scales limits the range of flame conditions that can be modeled (Maas & Pope, 1992). IDLM works best with reactions that always progress to equilibrium, but it falls short in scenarios such as extinction and re-ignition where the faster reaction rates are affected by the turbulent characteristics. Another promising method designed to handle the complex chemistry needed for reactive DNS studies is the In Situ Tabulation (ISAT) method, where the chemical source values at a given state are stored in a dynamically constructed table. With the ISAT procedure, the state vector is represented using a binary tree, and the chemical source terms are stored for recently performed calculations (Pope S., 1997). Later in the computation, when the same state conditions are encountered again, the calculations can be skipped in lieu of a table lookup. As expected, this procedure works best with problems where local equilibria are predominant. While these methods provide excellent options for capturing more detailed chemical compositions, they come with a cost: the limitations resulting from assumptions and bounding conditions. As stated before, each method tends to improve the solution capacity in one way by restricting it in others.

In addition to developments in the handling of chemical source terms, high-performance computing methods and parallel architectures have been investigated in great detail to expand the capabilities of DNS. Traditionally, the decomposition needed for parallel computation has been executed by breaking the larger domain up into smaller domains that
can be solved simultaneously. Each domain split provides the possibility to perform internal calculations twice as fast, but each split also adds an additional boundary. Handling these artificially added boundaries adds overhead with the data transferred between the nodes, as well as in the numerical calculations with boundary nodes. Parallelization studies continue to reach new levels of decomposition through adding thousands more nodes to the computational domain (Durst & Schafer, 1996; Laizet, Lamallais, & Vassilicos, 2010). These additions are not cheap, however, as the addition of each node carries a geometric increase in cost. New parallelization technologies make these additions more affordable, but the architectures are less applicable to direct decomposition. Parallelization hardware such as the GPGPU requires modifications to the numerical algorithm to best fit the hardware capabilities. Alternate views of DNS such as the Lattice-Boltzmann Method have a numerical structure that tends to be quite expensive with traditional hardware architectures. Viewing the domain in terms of individual particles, however, makes it a much better fit for the GPGPU structure (Rinaldi, Dari, Venere, & Classe, 2012). Using this approach has a great deal of promise; however, the GPGPU architecture having generic applicable designs is still forthcoming. Even though these studies combined with improvements in hardware and networking continue to expand the capacity of what DNS models can capture, they are still limited with regard to domain size, chemical reaction complexity, and solution applicability. Likewise, large-scale computing systems are expensive to build and carry a high operating cost, thus even with the many improvements in model scale and efficiency, other alternatives continue to be investigated.
1.3 DNS Alternatives

With the end goal of finding a solution method for turbulent flows that is not constrained by domain size or Reynolds number, two general methodologies have evolved over time: averaging and filtering. Both reduce the limitations on Reynolds number by reducing the scale differences represented in the running solution. Averaging reduces the scale differences by replacing fluctuating quantities with mean quantities; filtering removes the scale differences in a more direct way by simply filtering the small scales out of the solution. The predominant averaging technique is the Reynolds Averaged Navier-Stokes (RANS), where the Navier-Stokes equations are averaged either in time or via an ensemble (Veynante & Poinsot, 2005). Although the averaging process smears the data, eliminating important parts of the solution, RANS tends to be used to model designs because it is cost-effective and easily accessed through commercial software. The predominant filtering technique is the Large Eddy Simulation (LES), where either an explicit or implicit filter is applied to the Navier-Stokes equations (Veynante & Poinsot, 2005). Most solutions use an implicit filter, which is accomplished via the resolution of the LES grid, but some authors believe that explicitly filtered LES is more accurate. LES solutions are truly time-dependent and represent the large scales within a domain in the same fashion as a DNS solution would. For this reason, LES is more accurate for many problem types and represents the physics of a problem better than RANS; however, LES does require a higher computational cost. Furthermore, solving the closure problem is sometimes more complex with LES. For both RANS and LES, the focal point of modern research is the method by which information removed from the reduction mechanism is represented in the overall solution. Representing this lost information is considered the closure problem and is the focus of much of the research today. As mentioned
above, the complex relationship between turbulent motion and combustion is difficult to capture with any type of numerical solution. This difficulty is especially true within reduced scale mechanisms that cut out the very portions of the solution where the combustion is occurring. For this reason, many different methods have been investigated to solve this part of the closure problem. Some have persisted, some have not.

Several major approaches have been developed for resolving the closure problem associated with RANS and LES solutions to turbulent reacting flows. The majority of these methods were first developed for RANS and then later extended to LES. The extension is natural because, even though RANS and LES differ in how the reduction is defined, the resolved equations for each have similar forms. The differences stem from contrasts between an averaging function and a filtering function, which cannot be taken lightly. As a result, comparisons between each model must consider the necessary assumptions closely before expanding to more general problem spaces. Many of these closure methods fall into one of three main categories: sample space, PDF transport, and reduced dimensional stochastic models. While different in construction and formulation, each method has a similar object of representing the information residing in the scales smaller than the LES grid with a tractable, accurate solution. Each method is challenged by issues specific to the particular formulation, and how these problems are handled determines the resulting success.

1.4 State-Space Models

State-space models, starting with the flamelet model, were some of the earliest developed because they follow the traditional assumption that flames within a turbulent flow are fast and occur at scales much smaller than the Kolmogorov scale. This separation of scales
facilitates the treatment of flamelets strictly within the sub-grid domain, allowing them to be solved in state-space independently. The concept of scalar dissipation is then included to describe how the flamelets are manipulated by the turbulent flow properties (Peters, 2000; Williams, 1985). The flamelets can be solved as a function of a conservative state variable such as mixture fraction, and thus the solution can be closed by transporting this conservative variable within the spatial domain. A good example of this method is seen in the Lagrangian Flamelet Model study by (Pitsch & Steiner, 2000). The Lagrangian Flamelet Model represents the necessary closure problem by solving the unresolved state variables (species mass fractions and temperature) as functions of the mixture fraction. The filtered quantities are then calculated by integrating each unfiltered variable over a scalar probability density function (PDF), such as the β-PDF applied within the mixture fraction space. Unfortunately, this method has several limiting factors. First, the flamelet equation is based on the laminar flamelet assumption, which requires an additional component to capture the flame-turbulence interaction in order to close the solution completely. This phenomenon is normally captured by the addition of a scalar dissipation term within the flamelet solution. Once added, the problem is much more complex because the scalar dissipation must either be matched to the turbulent solution or modeled by some other means. The treatment of the scalar dissipation within the resolved domain is also quite a challenge because of its definition. Within the resolved domain, the scalar dissipation is a filtered quantity; however, within the state-space, an instantaneous or unfiltered quantity is required. Complex modeling, which is sometimes in the form of another PDF, is thus required to close these equations completely. In addition to the difficult treatment of the scalar dissipation, the β-PDF is an estimate, which is sometimes crude, of the actual distributions that are hidden within the turbulent behavior of each
conservative and reacting scalar. For flows that exhibit extinction and re-ignition, the $\beta$-PDF is not able to capture all the scalar distributions present accurately. Finally, the scale separation assumption limits the problem to a small class of flames where the flames are thinner than the smallest scales in the flow. Despite all these challenges, the flamelet model is still widely used and continues to draw attention in studies applying LES to represent turbulent reactive flows numerically. This popularity is mostly due to the simplicity and the wide spread adoption among commercial CFD codes.

An extension of the flamelet model is the conditional moment closure (CMC) method, where the solutions to the secondary state variables are solved as conditional averages within the mixture fraction space. This method assumes that fluctuations of the reactive scalars about the distribution of a conditioning variable (e.g., the mixture fraction in non-premixed combustion) are negligible. Resolved reactive scalars are determined selectively based on a solution in the state-space and a given distribution of a conserved scalar (Klimenkoa & Bilger, 1999). Having the state variables represented as conditional distributions minimizes issues associated with joint PDFs in the final integration of filtered quantities and reduces the overhead associated with treatment of turbulent-combustion interactions. It does not, however, relax the scale separation assumption. The more significant challenge with CMC methods is the use of assumptions concerning the shape of the PDFs to describe the relationship between conservative and non-conservative variables. Having to include assumptions on the shape of these PDFs places strong restrictions on the boundary conditions and limits the flexibility of each solution. CMC methods are still viable, however, due to the reduced computational overhead. Transporting conditional averages can be accomplished with much more coarse grids, thereby reducing the computational cost. (Garmory & Mastorakos, 2013) confirmed this
assessment with a study on how sensitive the CMC methods are to the LES grid. With the scalar dissipation being an exception, all of the conditional variables appeared to be insensitive to grid resolution. This finding is consistent with other known issues in dealing with the filtered scalar dissipation term.

1.5 PDF Transport Method

Due to limitations related to the scale separation assumption, the PDF transport method has emerged as one of the front runners in sub-grid closure models. As early as the late 1960s and 1970s, Lundgren and Pope determined that the combination of a scalars defined in composition space with a joint PDF describing the current state of the system is a viable method to solve RANS and LES equations without any unclosed terms. The next step in this progression is the derivation of equations transporting one or two of these PDFs, thus describing the states of the system within a turbulent flow (Lundgren, 1969; Pope S.B. , 1976). These methods were initially presented in theory only because the high dimensionality of the multivariate PDF leads to highly complex system that is to this day intractable. This condition remained until Monte-Carlo methods for solving these equations were introduced in the 1980s. PDF transport methods take advantage of a statistical observation that any turbulent or chemical system can be represented as a joint PDF between the overall solution state and the turbulent velocity. This PDF can be initialized with either a known or prescribed distribution and then be transported within the general solution space. Necessary information for closing averaged values is calculated as a function of the state PDF thus giving a complete view of the system (Pope S. B., 1985). While the distribution functions are considered complete and the transport equations are essentially closed, these methods still require additional effort to deal
with the turbulent fluctuations and how they affect the distribution. This challenge is evident in the expansion and development of the many different mixing models used to close the turbulent portions of the PDF transport equation (S. Viswanathan, Wang, & Pope, 2011). The most distinct challenge with PDF methods has to do with the computational cost of a direct solution to the PDF transport equation. The computational cost of a direct solution is higher than feasible because the joint PDF is based on a significant number of dimensions making it intractable in current computational space. Researchers instead have turned to stochastic methods such as the Lagrangian Monte Carlo method to solve the PDF transport equation in the spatial domain (Colucci, Jaberi, Givi, & Pope, 1998). While this method is good, a strategy is needed to manage the errors that result from using a finite number of particles within the Lagrangian transport process. As particles are transported within the solution, the overall state is a combination of each of the particles within a computational cell, which means that empty cells are a possibility. This situation must be avoided because it would represent a discontinuity.

More recent applications of PDF transport methods in LES closure require that a filtered density function (FDF) be used to represent the state of the system. In most cases, the FDF is viewed as a filtered PDF, where the PDF is a fine-grained density much like that used with RANS (Haworth, 2010). This combination causes issues where there is a filter applied to an ensemble average and vice versa. In his analysis of current research applications of FDF methods, (Haworth, 2010) also points out that these FDF methods are dependent on the selected filter, and that moments should be handled with care. This situation is partially mitigated by using a marginal filtered PDF, which is different from the FDF. Having the PDF separate from the filter eliminates the issues mentioned above which arise due to differences
between averaging and filtering. Needless to say, the solution methods must still take advantage of complex stochastic methods to close the final transport equations.

One novel application combines the physics represented in the laminar flamelet with the PDF obtained through transported distributions (Wang & Chen, 2005). This method applies the flamelet concept as above, but the PDFs used to calculate the filtered/averaged quantities are those transported using the Monte-Carlo solution for the joint scalar/velocity PDF. This approach simplifies the PDF transport equations by only including the PDF for the mixture fraction and the TKE transfer rate. Assuming that there is enough information in the fluctuations of these two terms to account for both scalar mixing and turbulent motion, these transported PDFs combined with the flamelet models are all that is required to close the LES solution. Historically, the filtered/averaged scalar dissipation rate has been difficult to describe, leading to the inclusion of an assumed PDF for the scalar dissipation rate (Pitsch & Steiner, 2000). Alternatively, this Flamelet-PDF method proposes an algorithm to construct the scalar dissipation rate distribution from the mixture fraction and the TKE transfer rate which are resolved via the PDF transport method. Unfortunately, the issues associated with Monte-Carlo transport equation solvers are still challenges in addition to the limitations due to the scale separation assumption.

1.6 Reduced Dimensional Models

Another alternative method to relax the scale separation assumption is one where the turbulent combustion problem is solved directly within a domain of reduced dimensions. Reduced dimensional models start by solving the spatially resolved Navier-Stokes equations for turbulent reactive flows in a one-dimensional domain. With the solution emulating a three-
dimensional problem, the stirring that results from turbulence must be simulated via a stochastic model. Both (Linear Eddy Model) LEM and (One-Dimensional Turbulence) ODT use the “maps” concept to simulate stirring events which discretely model turbulent flow patterns. These mapping events are dependent on a probability of selecting a random location at a given time with a likely size and shape (Kerstein A., 1999). Both simulations are driven by an eddy rate that determines this probability; however, they differ in the complexity of the rate calculation. LEM uses empirically determined constants while ODT uses a coupling based on transported flow properties. Realizations from LEM and ODT solutions generally contain the composition detail for a given state which also implicitly includes all of the necessary statistical information. Closure methods are at liberty to choose how to capture the statistical information and provide a working model accordingly. Early usage of these methods uses a prescribed probability distribution to determine the likelihood of a given filtered state, but recent developments have taken advantage of the implicit distributions resulting from PDF’s condition on filtered state variables (Ranganath & Echekki, 2008; Sankaran, Drozda, & Oefelein, 2009).

ODT is a natural fit for solutions that directly couple LES or RANS with a running sub-grid model because the ODT domain is finely resolved. Such an implementation has been demonstrated in the works of (Cao S., 2006), where a one-dimensional ODT solution is coupled with a three-dimensional LES solution simultaneously. In Cao’s study, the multiple ODT solutions are carried out along key portions of the LES domain, and solution information is exchanged between the ODT solutions and the LES domain during at each LES time step. This type of coupling has huge potential for LES closure models because it eliminates issues with determining the statistical distributions embedded in the data. Similarly to PDF transport
methods, implementations that support detailed chemistry models have potential limitations in the available computational infrastructure needed to provide an ideal performance.

Considering the methods discussed thus far, it is apparent that continued research is valuable to making each approach more robust and effective. Also, because these methods are mature enough to warrant industrial use, they frequently appear as extensions to commercial software. Regardless of adaptation, each method can benefit from improvements and enhancements to the models and implementations. Many of the recent advancements with these models include solutions for new problem spaces that have yet to be solved, and during these implementations, the new findings are then used to enhance the models further. This statement is true mostly for flamelet and PDF transport models where the methods are very mature and tend to be seen as the better choices for select problem domains. On the other hand, low-dimensional models have yet to reach all of the potential available. Thus, in addition to research expanding the use of low dimensional models, researchers continue to explore the untapped information that can be extracted from these simulations.

Reduced dimensional models are gaining more attention and acceptance because the methods eliminate much of the empirical nature seen in many of the other models, while still providing a computationally tractable alternative. The two basic implementations providing LES closure via ODT/LEM are integrated solutions and stand-alone solutions. Integrated solutions such as the Cao research solve the ODT solution alongside the LES solution, involving a large computational overhead. Stand-alone solutions solve the problem in the ODT domain and then provide closure via a table lookup or non-linear regression. While there is overhead in running the stand-alone ODT solution, the LES runtime savings are much more significant. With advancements in parallel architectures, integrated solutions will soon become
choice implementations; however, tabulation methods still have their place in future developments. Stand-alone methods offer a high degree of runtime simplicity with a smaller up-front investment, and they have the ability to interchange reaction mechanisms with little changes to the integrated model. Much of the new research required for coupled solutions involves the coupling mechanism between LES and ODT and improved efficiencies in the implementation. The interchange of information between these two solutions is paramount to the effectiveness of the method. Variables in the LES space require increased resolution, while information obtained from ODT requires reduced resolution. The difference introduces unnecessary error which may affect the outcome. In contrast, within the tabulation space, the biggest concern is finding an effective and efficient mechanism to represent the statistical nature of the solution. These methods either encapsulate the statistics and the spatial information within the same constructs, or they separate the statistics and combine the model via an integration step. Accurately representing the statistical nature is essential to predicting unresolved quantities within highly turbulent reactive flows. With the many layers of complex information, modeling the statistics can be quite difficult otherwise.

1.7 Justification of ODT as a Closure Model

A discussion about the viability of ODT must begin with a basic explanation of LEM and a description of the science behind the model. The key physics that an LEM simulation intends to capture are the effects of turbulent mixing on diffusive processes. The length scales along the turbulent cascade vary from the largest to the smallest, where the smallest also coincide with those length scales matching molecular diffusion and combustion processes. Within a turbulent mixing model, the first objective should be to emulate the transfer of energy
from the largest scale to the smallest. Reviewing a log of energy (log(E(k))) vs. wave number
k plot reveals that the wave number increases linearly as the energy is transferred downward
in the inertial range. This energy is then dissipated sharply beyond a certain wave number at
or below the Kolmogorov scale.

![Log-log plot of Energy Spectra](image)

**Figure 1.1** Log-log plot of Energy Spectra (Rebollo & Lewandowski, 2014)

The general idea behind the mixing model applied in LEM is that the transfer of
information across the inertial subrange is accomplished by incrementally increasing the wave
number on which the data distribution representing transported scalars resides. By matching
the information within the added frequencies to the linear effects of a turbulent eddy, LEM can capture both the motion and signal characteristics of turbulence in a single operation.

At the core of an LEM model is the triplet map, which is a very simple process that captures a linear representation of an eddy. It is a two-step process that involves both compression and rotation. The compression is accomplished by increasing the slope of the data and therefore reducing the length portion of the output signal. The modeling of rotation is achieved by flipping one-third of the data within the mapped region. The triplet map is thus a linear mechanism to represent the motion and statistical nature of the turbulent flow. The important thing to note is that the maps have the same effect as a turbulent eddy: they add additional frequencies, thereby reducing which length scales are more relevant in the modeled space. Over time, the length scales carrying important information are reduced to the smallest layer matching that of the molecular processes.

Albeit simple, the triplet maps which are at the core of LEM represent turbulent eddies quite well within a 1D domain. By transporting a three-dimensional velocity and using the resulting information to activate mapping events probabilistically, ODT further enhances this 1D representation of turbulence. ODT essentially removes the prescribed nature of eddy selection within LEM by using data present within the simulation. Much like turbulence in the physical domain, where the effects of each turbulent eddy are dependent on the preceding eddies, each eddy event within ODT is dependent on the turbulent motion leading up to it. This concept fits quite well with the time-marching algorithm within ODT simulations because the numerical operations for each time step are dependent on events from previous time steps. The convective events are dependent on previous statistics, and the diffusion and reaction processes are dependent on the results of convective motion.
A significant limitation with a 1D solution involves the orientation of the chosen domain. For many of the flows studied using ODT and LEM, the chosen domain is a cross section perpendicular to the dominant velocity pattern. For problem domains that involve a symmetrical or axisymmetric shear layer, this positioning of the 1D domain works quite well. (Echekki T., Kerstein, Dreeben, & Chen, 2001) provide several examples where a time-marching ODT solution for a symmetric channel or an axisymmetric jet can perform as well as a DNS solution given the proper boundary conditions. Unfortunately, in regions where the shear layer isn’t as well defined, selecting the placement of the 1D domain and the boundaries can be much more difficult. To overcome this challenge, models must account for more domains simultaneously, which is more difficult mathematically and computationally. In response to these challenges, coupled solutions model LES sub-grids via interlaced ODT domain. This type of approach enables application to a variety of domains, and expanding the number of applicable domains is vital to the growth of ODT research. Nonetheless, research continues to advance the traditional prescribed domain method because of its efficiency and reduced overhead.

1.8 Research Objectives

This research is focused on methods to extract and make use of as much of the information available within an ODT solution to create a more viable stand-alone closure model for LES. As stated above, ODT can be used to determine the correlations between dependent variables in a given state vector in a completed simulation. Furthermore, using the methods outlined by (Echekki & Kerstein, 1998), ensembles of ODT generated realizations provide a picture that is much like a 2D DNS rendition. Having this volume of data,
correlations extracted between filtered and unfiltered terms are a perfect source to build a filter density function. These constructed distributions provide a more realistic view of what PDFs are needed to build a state-based closure model that is an improvement over prescribed PDFs, such as the $\beta$-PDF. It follows that a stand-alone closure model can be built naturally by integrating over the ODT state-space with the extracted distributions. This combination of two separate aspects of the flow essentially reconstructs what was already present in the ODT solution, but in a form that is accessible via a filtered state vector. Models assembled in this fashion are validated via a known flow problems that have experimental data available for comparison. The ODT stand-alone model is validated using an LES solver built with OpenFOAM to simulate the Sandia piloted jet diffusion Flames.

1.9 Outline

The remaining chapters of this dissertation build a case for using information extracted from ODT simulations to determine all of the information needed to close an LES simulation of a turbulent non-premixed combustion problem. This case is supported first with Chapter 2 which explains LES methods covering in detail the justification of the closure method. Chapter 3 is both a review of ODT and a discussion of the solution characteristics that facilitate the data extraction needed for closure. Chapter 4 discusses extraction and processing of distribution and statistical data from ODT as well as construction of filter density functions based on kernel density estimates (KDE), and the final closure model applying ODT statistics. Then, Chapter 5 covers the application of this process to the Sandia Flames followed by analysis of ODT statistics and distributions. Finally, Chapters 6 and 7 discuss results from the
LES simulations of piloted jet diffusion flames, and Chapter 8 concludes with a discussion of the possible additions to the methodology covering future developments and considerations.
2 LES Governing Equations

2.1 Background for Non-Premixed Combustion LES

The derivation of LES governing equations starts with the resolved instantaneous conservation equations for a reacting mixture. Traditionally, Eulerian solutions to fluid problems start with the 3D formulation of the Navier-Stokes equations for compressible fluids (Peters, 2000). Within a closed aggregate system, where the fluid is treated as a statistical collection of particles, the Navier-Stokes equations describe the conservation of three key characteristics of the system: mass, momentum, and energy (Acheson, 1990). Conservation of mass captures the chemical and physical state of the fluid, which is comprised of a mixture of species components. The species component vector describes the individual species contributing to the mixture and provides access to many of the fluid properties such as viscosity, diffusivity and density. Momentum captures the results of a mass in motion. In the case of a mixture, momentum is the effect carried with the moving sum of all the transported species. The momentum equation is simplified by viewing the mixture as a sum of all the parts, which is the fluid density. Combining the fluid density with the directional velocity of the bulk fluid \((\rho u_i)\) gives a single view of the fluid momentum. Finally, the conservation of energy equation captures the potential, kinetic, thermal, and chemical energy within a system. For chemically reactive systems, these contributions all play a very complex role in the overall system.

Using an Eulerian view of the fluid, the instantaneous differential form of the conservation equations are as follows (Kuo, 2005):
\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (2.1)
\]

\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_k \frac{\partial Y_k}{\partial x_i} \right) + \omega_k \quad (2.2)
\]

\[
\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tau_{ij} \right) - \frac{\partial P}{\partial x_j} \quad (2.3)
\]

\[
\frac{\partial \rho h_t}{\partial t} + \frac{\partial \rho u_i h_t}{\partial x_i} - \frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_i} \left( u_i \tau_{ij} \right) - \frac{\partial q_i}{\partial x_i} + \sum_{k=1}^{N} \rho Y_k f_{ik} \cdot (u_i + V_{ik}) + \dot{Q} \quad (2.4)
\]

In Eq. (2.2), \( D_k \) is the diffusion coefficient of species \( k \) into the rest of the mixture, and \( \omega_k \) is the change in species \( k \) due to chemical reactions. \( \frac{\partial}{\partial x_i} \left( \tau_{ij} \right) \) represents changes to the momentum due the viscous forces within the fluid, and for Newtonian fluids this term can be written in terms of a stress tensor which captures changes in the fluid due to shear forces (Kuo, 2005).

\[
\frac{\partial}{\partial x_i} \left( \tau_{ij} \right) = \frac{\partial}{\partial x_i} \left( 2\mu \left( S_{ij} - \frac{1}{3} \delta_{ij} S_{kk} \right) \right) \quad (2.5)
\]

where

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.6)
\]

Here, \( \mu \) is the fluid viscosity, \( \delta_{ij} \) is the Kronecker delta, \( S_{ij} \) is fluid stress tensor, and \( S_{kk} \) is the trace of the fluid stress tensor, which is due to changes in the volume. Finally, the conservation of energy is expressed in terms of total enthalpy because it accounts for both the mechanical
and chemical changes in the fluid. In Eq. (2.4), $\frac{\partial}{\partial x_i} (u_j \tau_{ij})$ is the dissipation due to viscous forces, $\sum_{k=1}^{N} \rho Y_k f_{ik} \cdot (u_i + V_{ik})$ is the result of body forces within the fluid, and $\dot{Q}$ is the heat added to the system. $\frac{\partial q_i}{\partial x_i}$ contains changes due to heat transfer which include conduction, diffusion and Dufour effects. A key aspect of the LES method that makes the governing equations more robust than the corresponding DNS method is the application of a spatial filter. This filter limits the solution to a manageable range of data frequencies, but it also adds additional complexities to the solution. In order to minimize these complexities several steps are taken to simplify Eqs. (2.1) through (2.4) prior to filtering.

2.2 Mixture Fraction

Each of the transport equations for species mass fraction expressed in Eq. (2.2) includes a non-linear source term ($\omega_k$) which, as described in the next section, requires a model to close the equation completely. In addition, transporting this many equations can add complexity and overhead to the overall solution. Thus, a helpful and necessary step in the derivation of the LES transport equations is to reduce Eq. (2.2) to a single conserved scalar, which represents the composition of the entire fluid mixture. Using a conserved scalar in combination with the temperature, the species mass fractions can later be calculated through a post processing closure model. In general, any conserved scalar will work, but for non-premixed reacting flows, the value of choice is the mixture fraction. The mixture fraction provides a normalized view of a multi-component mixture with respect to a fuel stream and an oxidizer stream. It is the percentage of a mixture that is occupied by the fuel which can be used to show the mixing that leads to combustion and the state within post combustion products. In general, mixture
fraction can be expressed in terms of fuel and oxidizer stream mass fractions, but for complex mixtures using elemental mixture fractions works best.

Equation (2.7) was introduced in (Bilger, 1988) as a universal expression for mixture fraction. Being comprised of all of the elemental mixture fractions, this equation is valid for all mixture compositions regardless of the number of species.

\[
Z = \frac{\frac{2(Z_C - Z_{C,0})}{W_C} + \frac{1}{2} \left(\frac{Z_H - Z_{H,0}}{W_H} + \frac{Z_O - Z_{O,0}}{W_O}\right)}{\frac{2(Z_{C,f} - Z_{C,0})}{W_C} + \frac{1}{2} \left(\frac{Z_{H,f} - Z_{H,0}}{W_H} + \frac{Z_{O,f} - Z_{O,0}}{W_O}\right)}
\] (2.7)

In Eq. (2.7), the elemental mixture fractions are the sum of the contributions from each of the mass fractions present that contain the element.

\[
Z_j = \sum_{i=1}^{N} \frac{a_{ij} M_j}{M_i} Y_i
\] (2.8)

Using the expression in Eq. (2.7) to reduce Eq. (2.2) to a mixture fraction transport equation can be quite difficult. To simplify this process, the mixture fraction defined via elemental mixture fractions can be reduced to an equation in terms of fuel and oxidizer mass fractions. This transformation starts with a theoretical reaction in terms of fuel and oxidizer leading to a product.

\[
F + O = P
\] (2.9)

Considering \(CH_4\) and \(O_2\) as the fuel and oxidizer respectively, the above expression can be written as a single step methane + oxygen reaction.

\[
CH_4 + 2O_2 = CO_2 + 2H_2O
\] (2.10)
The mass fractions from the fuel-oxidizer equation -- Eq. (2.9) -- and the methane reaction -- Eq. (2.10) -- are defined as $Y_F = Y_{CH_4}$ and $Y_O = Y_{O_2}$. With these definitions, the elemental mixture fractions can also be expressed in terms of a fuel and oxidizer mass fraction: $Z_C = \frac{M_C Y_F}{M_F}$, $Z_H = \frac{4M_H Y_F}{M_F}$ and $Z_O = \frac{4M_O Y_O}{M_O}$. To continue, a single conserved scalar, $\beta$ in terms of $Z_C$, $Z_H$ and $Z_O$ is defined.

$$\beta = \frac{Z_C}{M_C} + \frac{Z_H}{4M_H} - \frac{Z_O}{2M_O}$$  \hspace{1cm} (2.11)

After substituting the expressions for elemental mass fraction, $\beta$ can be expressed in terms of species mass fractions.

$$\beta = \frac{Y_F}{M_F} + \frac{Y_F}{M_F} - 2 \frac{Y_O}{M_O}$$

$$\beta = 2 \frac{Y_F}{M_F} - 2 \frac{Y_O}{M_O}$$

$$\beta = Y_F - \frac{M_F}{M_O} Y_O$$

$$\beta = 2Y_F - 2 \left( \frac{F}{O} \right)_{st} Y_O$$  \hspace{1cm} (2.12)

The solution mixture fraction is defined in terms of $\beta$ for the mixture, $\beta^F$ for the fuel stream and $\beta^O$ for the oxidizer stream.

$$Z = \frac{\beta - \beta^O}{\beta^F - \beta^O}$$  \hspace{1cm} (2.13)

For the fuel stream $Y_F = 1$, and for the oxidizer stream $Y_O = 1$; thus $\beta^F = 2$ and $\beta^O = -2 \left( \frac{F}{O} \right)_{st}$. Equation (2.13) can be expressed in term of fuel and oxidizer mass fractions.
\[ Z = \frac{2Y_F - 2 \left( \frac{F}{\Omega} \right)_{st} Y_O - \left( -2 \left( \frac{F}{\Omega} \right)_{st} \right)}{2 - \left( -2 \left( \frac{F}{\Omega} \right)_{st} \right)} \quad (2.14) \]

If \( \left( \frac{F}{\Omega} \right)_{st} = 1 \) as before, then Eq. (2.14) can be simplified to the following.

\[ Z = \frac{2Y_F - 2Y_O + 2}{2 + 2} = \frac{1}{2} [1 + Y_F - Y_O] \quad (2.15) \]

The final expression, Eq. (2.15) is then be combined with the species transport Eq. (2.2) to form an equation for the mixture fraction.

\[
\frac{\partial \rho Y_F}{\partial t} + \frac{\partial \rho u_j Y_F}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_k \frac{\partial Y_F}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \rho D_k \frac{\partial Y_O}{\partial x_j} \right) + \omega_F - \omega_O \quad (2.16)
\]

In Eq. (2.16) the sum of the source terms are equal to zero \((\omega_F = \omega_O)\), the derivative of a constant is equal to zero, and the species diffusion coefficients are assumed equal. Thus, the transport equation for the mixture fraction reduces to the following.

\[
\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_j Z}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_z \frac{\partial Z}{\partial x_j} \right) \quad (2.17)
\]

It is important to note that there is no longer a chemical source term because ultimately conserved scalars have neither sources nor sinks. This elimination will be very helpful later once the filtering process is completed as it eliminates a non-linear source term. Likewise, the diffusion coefficients have been reduced to a single, non-dimensional coefficient \( D_z \) which can later be related to the fluid viscosity.
2.3 LES Momentum

The transformation of the conservation equations into the LES domain requires application of a spatial filter to cut off the high-frequency (or small-scale) contributions (McDonough, 2007). This filtering process appears as an integration, applying a filter function over the spatial domain.

\[ \Psi = \int G(x_i - \xi) \psi(\xi) \, d\xi \]  

(2.18)

While any symmetrical filter kernel \( G \) will work, many times a Gaussian or Box filter is used for simplicity. The filtering operation is different from the averaging function used with RANS, but the two operations share enough properties to render similar governing equations. Namely, because both are expressed as integrals, both share the distributed property allowing each contribution to be filtered separately. The filtered version of Eq. (2.3) is listed below.

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tau_{ij} \right) - \frac{\partial P}{\partial x_i} \]  

(2.19)

Filtering a convolution such as \( u_j u_i \) is also similar to the averaging function because the term \( \frac{\partial \rho u_j u_i}{\partial x_j} \) results in a complex set of individual contributions when decomposed. The filtered advection term is not tractable; thus, further analysis is required to obtain an equation which is able to be solved. Again, much like the RANS averaging, the density can be separated using a Favre-averaged filtering which separates the filtered density from the filtered product. Favre-averaged filtering involves separating the filtered density from the filtered product by dividing the filtered product with the filtered density.

\[ \bar{\Psi} = \frac{\int G(x_i - \xi) \rho \psi(\xi) \, d\xi}{\int G(x_i - \xi) \rho(\xi) \, d\xi} \]  

(2.20)
Equation (2.20) is simplified by expressing the integral in terms of the filter notation.

\[ \bar{\Psi} = \frac{\rho \Psi(\xi)}{\bar{\rho}} \]  

(2.21)

A simple manipulation of Eq. (2.21) leads to the natural expression \( \bar{\rho} \bar{\Psi} = \rho \Psi(\xi) \) which can be substituted into Eq. (2.19) resulting in the following form for the momentum equation.

\[ \frac{\partial \bar{\rho} \bar{u_i}}{\partial t} + \frac{\partial \bar{\rho} \bar{u_j} \bar{u_i}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tau_{ij} \right) - \frac{\partial \bar{P}}{\partial x_i} \]  

(2.22)

The next step is to express \( \bar{u_j} \bar{u_i} \) in terms that can be explained through alternate means. The term \( \bar{u_j} \bar{u_i} \) can be expanded to \( \bar{u_j} \bar{u_i} = \bar{u_j} \bar{u_i} - \bar{u_j} \bar{u_i} + \bar{u_j} \bar{u_i} \) which can then be substituted into Eq. (2.22).

\[ \frac{\partial \bar{\rho} \bar{u_i}}{\partial t} + \frac{\partial \bar{\rho} \bar{u_j} \bar{u_i}}{\partial x_j} = - \frac{\partial}{\partial x_j} \rho (\bar{u_j} \bar{u_i} - \bar{u_j} \bar{u_i}) + \frac{\partial}{\partial x_j} \left( \tau_{ij} \right) - \frac{\partial \bar{P}}{\partial x_i} \]  

(2.23)

The expression \( (\bar{u_j} \bar{u_i} - \bar{u_j} \bar{u_i}) \) is formally termed the sub-grid stress, and it represents the viscous dissipation of turbulent energy at scales below the filter size. Without a direct solution, this expression must be modeled such that it can be resolved with known quantities.

The sub-grid stress, \( \rho (\bar{u_j} \bar{u_i} - \bar{u_j} \bar{u_i}) \), is assumed to follow a dissipative character and can be modeled in terms of the large scale strain-rate. More formally, this can be expressed using an SGS-eddy viscosity (Ferziger, 1996):

\[ \bar{\rho} (\bar{u_j} \bar{u_i} - \bar{u_j} \bar{u_i}) \equiv \bar{T}_{ij} \approx -2\mu_{SGS} \bar{S}_{ij} \]  

(2.24)

where \( \bar{T}_{ij} \) represents the eddy-viscosity SGS stress term, \( \mu_{SGS} \) is the perceived viscosity due to turbulent dissipation, and \( \bar{S}_{ij} \) is the filtered result of Eq. (2.6). As stated above, the physical description of the SGS stress term is the energy dissipated below the Taylor microscale length.
In a numerical sense, the SGS stress provides the numerical dissipation needed to make a coarse-grained solution more stable. The SGS-eddy viscosity $\mu_{SGS}$ must relate the available energy to the possible dissipative character of the flow, and thus it must be modeled using concepts relating the available flow energy to a viscosity. If all the available energy is assumed to be dissipated via this eddy viscosity then, the SGS viscosity can be modeled in direct relation to the magnitude of the shear stress.

$$|\tilde{S}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$$ (2.25)

What remains is an expression that captures the size of the filter used to remove this lost information. As seen in the next section, including the LES filter size in the definition of the SGS viscosity quantifies the detail lost.

### 2.4 Smagorinsky Model and Momentum Closure

In the 19th Century, Boussinesq proposed that the turbulent stress seen in Eq. (2.24) is proportional to the velocity gradient, much like the stresses seen in laminar flow. This idea likens the eddy viscosity to the mixing length, which is related to the magnitude of the stress tensor. (Smagorinsky, 1963) formalized this theory for LES by considering that the filter width is also related to the mixing length, thus contributing to the exhibited turbulent stresses. With these ideas, the SGS viscosity is considered to be proportional to the magnitude of the shear stress and the filter width (McDonough, 2007).

$$\mu_{SGS} = 2C_s^2 \Delta^2 |\tilde{S}|$$ (2.26)

Unfortunately, this approach has several limitations, such as a tendency toward excessive dissipation and the inability to capture changes in flows bounded by walls; however, it
performs reasonably well in free-flowing jets with known levels of turbulence. As a result, this approach is a decent choice for a round jet surrounded by a free stream. The dissipation issues and flexibility can be relaxed with a formulation that determines $C_s$ dynamically, but this approach adds a considerable degree of computational overhead. For selective problems, a fixed constant may be desirable due to the simplicity and limited variability in the shear layer.

Looking again at the filtered momentum equation, the terms can be written such that the sub-grid stress is in the same form as the viscous force term.

$$\frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( 2\mu_{SGS} \left( \tilde{\Sigma}_{ij} - \frac{\delta_{ij}}{3} \tilde{\Sigma}_{kk} \right) \right)$$

$$+ \frac{\partial}{\partial x_j} \left( 2\mu \left( \tilde{\Sigma}_{ij} - \frac{\delta_{ij}}{3} \tilde{\Sigma}_{kk} \right) \right) - \frac{\partial \tilde{P}}{\partial x_i}$$

The viscous stresses from Eq. (2.27) can be combined to form a turbulent viscosity, which appears as a linear combination of the shear stress and the SGS stress.

$$\frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( 2\mu_{SGS} + 2\mu \left( \tilde{\Sigma}_{ij} - \frac{\delta_{ij}}{3} \tilde{\Sigma}_{kk} \right) \right) - \frac{\partial \tilde{P}}{\partial x_i}$$

(2.28)

While the contributions due to $\tilde{\Sigma}_{kk}$ can also be modeled, many times they are neglected because the contribution is minimal compared to the other terms (Kuo, 2005). The final version of Eq. (2.28) includes contributions due to advection, shear and SGS stresses, and the pressure.

$$\frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( 2\mu_T \tilde{\Sigma}_{ij} \right) - \frac{\partial \tilde{P}}{\partial x_i}$$

(2.29)
Equation (2.29) uses a turbulent viscosity, which is the combination of the fluid viscosity and the SGS viscosity term: \( \mu_T = \mu_{SGS} + \mu \). In a turbulent jet where the boundaries are defined without any no-slip boundary conditions, the SGS viscosity dominates the entire flow. With Eq. (2.29) in this form, any mixing model which is consistent with the eddy viscosity assumption can be used to calculate \( \mu_T \). This approach is covered in more detail in Appendix A1.

### 2.5 LES Scalar Transport Equations

After filtering the transport equation for mixture fraction, the filtered advection term also results in a sub-grid stress contribution.

\[
\frac{\partial \bar{\rho} \bar{Z}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{Z}}{\partial x_j} = -\frac{\partial}{\partial x_j} \bar{\rho} (\bar{u}_j \bar{Z} - \bar{u}_j \bar{Z}) + \frac{\partial}{\partial x_j} (\bar{\rho} D_t \frac{\partial \bar{Z}}{\partial x_j}) \tag{2.30}
\]

Applying a similar argument to the eddy viscosity, the SGS stress for scalars can be empirically determined from the scalar gradient.

\[
\bar{\rho} (\bar{u}_j \bar{Z} - \bar{u}_j \bar{Z}) = \rho D_t \frac{\partial \bar{Z}}{\partial x_j} \tag{2.31}
\]

In Eq. (2.31) \( D_t \) is an effective turbulent diffusivity, which follows the same pattern as that used with Smagorinsky model.

\[
D_t = C_D^2 \Delta^2 |\bar{S}| \tag{2.32}
\]

The turbulent diffusivity is related to the turbulent viscosity via the turbulent Schmidt number, which is the ratio of the fluid viscosity to the molecular diffusivity.
\[ D_t = \frac{\mu_{SGS}}{S_c} \]  \hspace{1cm} (2.33)

After combining the diffusive terms on the right hand side, Eq. (2.30) simplifies to the following.

\[ \frac{\partial \bar{\rho} \bar{Z}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{Z}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \bar{\rho} (D_z + D_t) \frac{\partial \bar{Z}}{\partial x_j} \right) \]  \hspace{1cm} (2.34)

Before discussing the filtered enthalpy equation, several assumptions must be clarified. As mentioned previously, in a non-premixed jet with only free stream boundary conditions, boundary layers are not present. Without any boundary layers, dissipation due to viscous forces is minimal in the present of turbulent motion and can be neglected. In addition, the body forces are assumed to be minimal and the only heat additions are from chemical reactions. Finally, the only heat-transfer effect considered is conduction. Applying Fourier’s law, the heat transfer term can be written as a function of the temperature gradient.

\[ \frac{\partial q_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) \]  \hspace{1cm} (2.35)

With these assumptions and a similar rationale to deal with the SGS stress equivalent as above, the filtered energy equation in terms of enthalpy is as follows.

\[ \frac{\partial \bar{\rho} \bar{h}_s}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{h}_s}{\partial x_j} - \frac{\partial \bar{p}}{\partial t} = \frac{\partial}{\partial x_i} \left( \left( \frac{\mu_{SGS}}{P_r} + \lambda \right) \frac{\partial T}{\partial x_i} \right) + \bar{\omega}_T \]  \hspace{1cm} (2.36)

In Eq. (2.36), the non-linear source term \( \bar{\omega}_T \) requires closure, and the turbulent Prandtl number is used to relate the SGS fluid viscosity to the sub-grid thermal diffusivity:

\[ P_r = \frac{\mu_{SGS}}{\alpha_T} \]
where $\alpha_T$ is the thermal conductivity associated with the SGS transport of the enthalpy. Relaxing the assumptions that lead up to Eq. (2.36) is possible when supported by more advanced CFD applications. Topics related to heat transfer and radiation are covered in more detail in Appendix A6.

The solution comprised of Eqs. (2.36), (2.34), and (2.29) is completely closed by solving the pressure gradient and modeling the chemical source term and density. The pressure gradient is solved using the pressure correction method, which is described in the next section, and the chemical source term and density are determined from LES closure. These topics are expanded in Sections A4 and 2.6. Also, an important detail to note concerning Eq. (2.36) is that the chemical source term and density are closed in terms of the temperature. With the energy expressed in terms of enthalpy, the solution must also solve for the temperature each time Eq. (2.36) is solved. Appendix A8 covers the method by which this calculation is accomplished.

### 2.6 Density and Chemical Source Term

The final unclosed terms are the filtered density and chemical source contribution for the filtered energy transport equation. By solving for the filtered density using a closure function, Eq. (2.1) can be eliminated, which is equivalent to replacing the species conservation equation with an equation of state. Unlike an equation of state using a filtered state variable, using LES closure for the density takes into account the sub-grid nature of the solution. The filtered density and chemical source term are functions of filtered quantities within the LES domain as well as other supporting variables.
\[
\bar{\rho} = \rho_{cls}(P, Z, T, \ldots)
\]  
(2.37)

\[
\bar{\omega} = \omega_{cls}(\bar{Z}, \bar{T}, \ldots)
\]  
(2.38)

\(\rho_{cls}\) and \(\omega_{cls}\) represent the density and chemical source term from LES closure respectively, and the filtered pressure is included in the function for density to keep the solution consistent with an equation of state. This connection is covered in more detail in Appendix A4. What remains is the problem of describing a function for a filtered variable in such a way that the sub-grid processes are captured accurately, having only filtered inputs. As stated in the introductory chapter, this problems is solved by combining information about the spatially resolved dependent variable in state-space and a distribution that describes the behavior of the state variable in filtered space.

## 2.7 LES Closure with Filter Distribution Function

Applying the properties of a probability distribution function (PDF), a statistical average can be described as the integral of the PDF and the dependent variable over the space of the distribution (Faber, 2012).

\[
\langle \varphi(\eta) \rangle = \int_{-\infty}^{\infty} \varphi(\eta)P(\eta)d\eta
\]  
(2.39)

Here \(\eta\) is the state variable, \(\varphi(\eta)\) is the dependent variable and \(P(\eta)\) is the distribution. The distribution is a functional representation of the likelihood that an instantaneous value of \(\eta\) contributes to the averaged value of \(\varphi(\eta)\). A similar correlation can be drawn for filtered
quantities by defining the filter distribution function (FDF) similarly to the PDF (Colucci, Jaberi, Givi, & Pope, 1998).

\[
\overline{\varphi(\eta)} = \int_{-\infty}^{\infty} \varphi(\eta) F(\eta) \, d\eta
\]  

(2.40)

\(F(\eta)\) is the statistical likelihood that a spatially resolved value of \(\eta\) contributes to the filtered value of \(\varphi(\eta)\). Append D1 provides additional background information on PDFs and FDFs. From here on, unless explicitly stated, \(P(\eta)\) is used to represent an FDF within equations.

While FDF and PDF profiles appear similar, they are very different in concept. Both predict the likelihood that a value in one space contributes to the result in another, but the differences affect how the functions can be manipulated and how the distributions are obtained (Haworth, 2010). Mathematically, they are treated the same, which allows for drawing many of the same conclusions for LES closure as with RANS. With a functional description of a distribution, the minimum requirements are the statistical mean and some measure of statistical width or range. The second moment of a distribution, which is commonly termed the variance, is a measure of the distance from the mean for all the contributions within a distribution.

Interestingly, within a turbulent dataset, the variance can also be an indicator of turbulent effects on the scalars described. An increasing variance is indicative of a scalar being “stretched” by the turbulent flow, while a decreasing variance shows the scalar being compressed more toward a laminar flow. With an FDF with the first and second moments included in the definition, a filtered value is expressed as a function of the instantaneous value, the filtered value and the sub-grid variance (Cook & Riley, 1994).

\[
\overline{\psi(\bar{Z},\bar{Z}'\bar{Z}')} = \int \psi(Z) P(Z, \bar{Z}, \bar{Z}', \bar{Z}'') \, dZ
\]  

(2.41)
The inclusion of second moments also requires that the variances be an integral part of the RANS or LES solution. Utilization of a closure method based on Eq. (2.41) must either calculate or transport the variance for each independent variable. For the many of the studies that do not use statistics based on reactive scalars, the variance for mixture fraction is modeled; however, in studies that do use the reactive scalar statistics, this type of approach is not sufficient (Jimenez, Ducros, Cuenot, & Bedat, 2001). These variances must be transported with the solution in order to more closely match the physical nature of the scalar within a turbulent flow. Another factor to consider in turbulent reactive flows is the functional dependence of the filtered density and chemical source on the filtered temperature. (Kronenburg, 2004) showed that the functional dependence on temperature cannot be neglected when calculating these dependent variables. By definition, this dependence results in a multivariate distribution $P(\bar{Z}, \bar{T})$ or a joint scalar FDF; however, if the mixture fraction and temperature are assumed to be statistically independent, the distributions can be separated: $P(\bar{Z}, \bar{T}) = P(\bar{Z})P(\bar{T})$. This separation is covered in more detail in Appendix D1. Adding temperature to the functional dependence of $\psi$, the definition of a filtered dependent variable includes joint scalar FDF and the resolved $\psi$ as a function of temperature and mixture fraction.

$$\overline{\psi(\bar{Z}, \bar{Z}^*, \bar{T}, \bar{T}^*)} = \iint \psi(Z, T) P(Z, \bar{Z}, \bar{Z}^*) P(T, \bar{T}, \bar{T}^*) dZ dT$$

(2.42)

Continuing with the objectives of the LES-ODT closure model, solving Eq. (2.42) requires spatially resolved statistics describing $\psi(Z, T)$ in state-space and filtered distributions for both mixture fraction and temperature.
2.8 Variance Transport Equations

For non-reactive scalars, (Peters, 2000) proposes that the sub-grid variance changes relative to the scalar dissipation. For the reason, the scalar dissipation has been chosen as the variable connecting the state-space with the instantaneous filtered space within an LES domain (Pitsch & Steiner, 2000). This similarity also enables representation of the variance algebraically using the square of the scalar gradient.

\[ \bar{Z}'^2 = C \Delta^2 |\nabla \bar{Z}|^2 \]  

(2.43)

This type of model works well for non-reactive conservative scalars due to the fact that only inputs affecting the scalar are due to the turbulent flow and molecular diffusion. With reactive scalars such as temperature and non-conservative mass fractions, representing the variance is more complicated because of the addition of the chemical source term. This non-linear addition causes the algebraic models to be less effective, requiring a more realistic model which can capture the effects of turbulence, diffusion and chemical reaction simultaneously.

By far, implementation of a transport equation for these variances is the best solution for capturing the complex combination of each of these effects. Unfortunately, the derivation and application of such a transport equation requires a simplification step relating the scalar variance to known filtered quantities. With the following expression for a scalar variance, a transport equation can be derived from the filtered scalar transport equation.

\[ \bar{T}'^2 = \bar{T}^2 - \bar{T}'^2 \]  

(2.44)

By re-writing Eqs. (2.4) and (2.36) in terms of temperature they can be manipulated and combined to derive a transport equation for the temperature variance. Equation (2.4) is
multiplied by 2T and filtered while Eq. (2.36) is multiplied by \( 2\tilde{T} \) resulting in the Eqs. (2.45) and (2.46) respectively (Jimenez, Ducros, Cuenot, & Bedat, 2001).

\[
\frac{\partial \bar{\rho} T^2}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j T^2}{\partial x_j} = \frac{\partial}{\partial x_i} \left( \bar{\rho} c_p \frac{\partial \bar{T}}{\partial x_i} \right) - 2\bar{\rho} \frac{\partial}{\partial x_i} \frac{\partial \bar{T}}{\partial x_i} - \bar{\rho} \frac{\partial}{\partial x_i} \left( \bar{u}_j T^2 - \bar{u}_j \bar{T}^2 \right) + 2\tilde{T} \omega_T \tag{2.45}
\]

\[
\frac{\partial \bar{\rho} \bar{T}^2}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{T}^2}{\partial x_j} = \frac{\partial}{\partial x_i} \left( \bar{\rho} c_p \frac{\partial \bar{T}}{\partial x_i} \right) - 2\bar{\rho} \frac{\partial}{\partial x_i} \frac{\partial \bar{T}}{\partial x_i} - 2\bar{\rho} \frac{\partial}{\partial x_i} \left( \bar{u}_j \bar{T}^2 - \bar{u}_j \bar{T}^2 \right) + 2\tilde{T} \omega_T \tag{2.46}
\]

After subtracting Eq. (2.46) from (2.45) several terms must be manipulate in order for the final version to be tractable. First, using the same logic to derive Eq. (2.44), the expression \( T''\omega_T'' \) can be defined in terms of the temperature and the chemical source terms.

\[
\bar{T''} \omega_T'' = \bar{T} \omega_T - \bar{T} \tilde{\omega}_T \tag{2.47}
\]

The non-linear stress terms follow a similar process to that used to derive the LES transport equation for mixture fraction and enthalpy.

\[
2T \frac{\partial}{\partial x_i} \left( \bar{u}_j T - \bar{u}_j \bar{T} \right) - \frac{\partial}{\partial x_i} \left( \bar{u}_j \bar{T}^2 - \bar{u}_j \bar{T}^2 \right) = \frac{\partial}{\partial x_j} \left[ \alpha_T \frac{\partial \bar{T''}}{\partial x_j} \right] + 2\alpha_T \frac{\partial \bar{T}}{\partial x_i} \frac{\partial \bar{T}}{\partial x_i} \tag{2.48}
\]
The second term in the RHS of Eq. (2.45) is considered the filtered scalar dissipation, of which there is no direct solution. Following the logic described by (Peters, 2000) the ratio of the scalar variance and the filtered scalar dissipation is proportional to the flow time which is in turn proportional to the ratio of kinetic and dissipated energy.

\[ \frac{\partial \bar{T}}{\partial x_i} \frac{\partial \bar{T}}{\partial x_i} = c_f \bar{T}^{\prime \prime 2} \frac{\tilde{\varepsilon}}{2k} \]

The final form of the temperature variance transport equation follows a similar form to the energy transport equation (Eq. (2.49)) with two additional source terms.

\[ \frac{\partial \tilde{\rho} \bar{T}^{\prime \prime 2}}{\partial t} = - \frac{\partial \tilde{\rho} \tilde{u}_j \bar{T}^{\prime \prime 2}}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \tilde{\rho} \alpha_T \frac{\partial \bar{T}^{\prime \prime 2}}{\partial x_j} \right] \]

\[ + 2 \tilde{\rho} \alpha_T \left( \frac{\partial \bar{T}}{\partial x_j} \right)^2 - \tilde{\rho} c_f \bar{T}^{\prime \prime 2} \frac{\tilde{\varepsilon}}{2k} + 2 \bar{T}^\omega \bar{T}^\omega \]

(2.49)

As with the other filtered equations discussed in this chapter, \( \bar{T}^\omega \bar{T}^\omega \) and \( \frac{\tilde{\varepsilon}}{2k} \) must be modeled, while \( \left( \frac{\partial \bar{T}}{\partial x_j} \right)^2 \) is calculated from the solution temperature. \( \bar{T}^\omega \bar{T}^\omega \) is modeled using a closure method similar to the chemical source term in Eq. (2.36) because it is constructed using the same ODT artifacts. Furthermore, the definition of \( \bar{T}^\omega \bar{T}^\omega \) includes the filtered chemical source term, and thus construction of \( \bar{T}^\omega \bar{T}^\omega \) requires knowledge of the filtered source. While \( \frac{\tilde{\varepsilon}}{2k} \) is sometimes modeled algebraically, if the turbulence model is implemented using complementary theories, it can be extracted from expressions internal to the turbulence implementation. This application, however, does not make the expression more accurate than
the algebraic expression. It only simplifies the computation of the term. This procedure is explained in more detail in Appendix A5.

The mixture fraction variance is also dependent on the energy balance, but does not have a chemical source term.

\[
\frac{\partial \rho \overline{Z} \overline{Z}^*}{\partial t} = -\frac{\partial \rho \overline{u}_j \overline{Z} \overline{Z}^*}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \bar{\rho} D_T \frac{\partial \overline{Z} \overline{Z}^*}{\partial x_j} \right] + \bar{\rho} 2D_T \left( \frac{\partial \overline{Z} \overline{Z}^*}{\partial x_j} \right)^2
\] + \bar{\rho} t \overline{Z} \overline{Z}^* \frac{\bar{\varepsilon}}{2k}
\]

(2.50)

Here the same logic applies to \( \left( \frac{\partial Z}{\partial x_j} \right)^2 \) and \( \frac{\varepsilon}{2k} \) as above where the quantities can either be modelled or extracted from solution artifacts.
3 ODT Background and Formulation

3.1 Background

A turbulent flow is comprised of eddies varying in size and position which give the appearance of independent random motions. However, when viewed as an ensemble, these motions converge into the larger scale motion where the velocity gradients prove to be the key aspects both visually and numerically. From the smallest viewpoint, the energy originating from the velocity gradients eventually dissipates at the molecular level, which also contains diffusion and combustion processes. This interaction of turbulent dissipation and molecular processes is very important with turbulent models that take advantage of the diffusive nature of most scalars by treating the energy dissipation as a turbulent diffusion mechanism. The challenge, then, is to account for the transfer of energy from the large scale motion to the molecular level in a tractable way in conjunctions with these other molecular processes. Kolmogorov’s illustration of the energy cascade within turbulence provides a good starting point for this discussion because it shows a continuous view of the energy transferred downward between these scales (Cushman-Roisin, 2014). In response, a good model for turbulent flows must capture all possible flow characteristics using the local properties of a given domain in order to predict stochastically the subsequent transfer of energy while also providing a solution at the molecular level. ODT is such a model. It uses the velocity gradients within the flow to “randomly” trigger discrete renditions of a turbulent eddy while simultaneously transporting a continuous reaction-diffusion mechanism (Kerstein A., 1992).
### 3.2 ODT Formulation

As stated previously, the intent of ODT is to make the compressible solution for chemically reactive fluids more tractable by reducing the dimensionality. Starting with the same logic and assumptions as seen in Chapter 2, the equations used to describe a chemically reactive turbulent flow are the conservation of mass, species, momentum and energy. Additionally, in the ODT formulation, the pressure is assumed to be constant and the mixture density is subject to the following equation of state:

\[ P = \frac{\rho R_u T}{W_M} \]  \hspace{1cm} (3.1)

In this form, \( R_u \) is the universal gas constant, \( W_M \) is the mixture molecular weight, and the density (\( \rho \)) is the sum of the partial densities of each species present in the mixture:

\[ \rho = \sum \rho_k \]

The change in momentum captures the effects of advection and forces on the bulk fluid (Acheson, 1990).

\[ \frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \tau_{ij} \right) - \frac{\partial P}{\partial x_j} \]  \hspace{1cm} (3.2)

In Eq. (3.2) \( \frac{\partial}{\partial x_l} \left( \tau_{ij} \right) \) is the same expression as that applied in Eq. (2.5). While the pressure also plays an important role in the momentum equation, the most complex contribution is the advection term, \( \frac{\partial \rho u_i u_j}{\partial x_l} \), which is a non-linear convolution between two different velocity vectors. This complexity is the root motivation for the ODT formulation. Next, the change associated with each species is considered.
\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_k \frac{\partial Y_k}{\partial x_i} \right) + \omega_k \quad (3.3)
\]

The species transport equations account for the changes in each species due to the fluid motion, the movement between each species (diffusion) and the chemical change of the system due to reactions. In Eq. (3.3) the species diffusion is expressed in terms of Fick’s second law which is best used with binary diffusion where the diffusion effects are equally balanced. In order to account for the differential diffusion associated with species such as Hydrogen, the diffusion term is best left in the form specified by Fick’s first law (Kuo, 2005).

\[
\frac{\partial}{\partial x_i} (\rho Y_k V_{ik}) = - \frac{\partial}{\partial x_i} \left( \rho D_k \frac{\partial Y_k}{\partial x_i} \right) \quad (3.4)
\]

Equation (3.4) leaves the diffusion velocity \(V_{ik}\) to be calculated numerically based on which method best fits the model. Finally, as stated before the conservation of energy is a combination of many different effects on the total energy of the system.

For simplification, a constant pressure adiabatic system neglecting the effects of radiation and any outside forces is assumed. Also, as described later in Section 2.5, the CHEMKIN library is used to calculate the chemical source terms. These routines are mostly written in terms of temperature and species mass fractions, so solving for the conserved total energy or enthalpy presents a challenge when calculating reaction rates and transport properties. With this approach the energy equation is best written in terms of temperature, which removes the conversion from enthalpy to temperature during each time step. With these assumptions, the conservation of energy in terms of temperature includes contributions from the fluid motion, heat transfer and the chemical reaction.
\[
\rho C_p \frac{\partial T}{\partial t} + \rho C_p u_i \frac{\partial T}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} - \dot{\omega} \quad (3.5)
\]

The heat transfer expression \(\left(\frac{\partial q_i}{\partial x_i}\right)\) includes contributions due to conduction and molecular diffusion.

\[
\frac{\partial q_i}{\partial x_i} = \rho \sum C_{pk} Y_{ik} \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i}\right) \quad (3.6)
\]

The diffusion velocities shown in Eqs. (3.4) and (3.6) are one and the same, which allows for reuse during computational iterations. These above described \(k+3\) equations comprise the necessary framework to represent a simplified fluid system mathematically leading to a discrete numerical solution. By solving this system of equations with given initial and boundary conditions, any fluid problem can be described with reasonable accuracy. Unfortunately, constraints due to the non-linear contributions render the problem difficult to solve, which is why alternatives continue to be investigated.

The derivation of ODT from the above described conservation equations starts with a discussion of each of the terms contributing to given transport equations. For the most part, each equation includes a source term, a diffusion term and an inertial term. The inertial term provides three main contributions to the fluid: bulk motion, stirring motion and the transfer of energy from one scale to the next (lower). The transfer of energy could be considered the result of stirring; however, when considering alternative methods to represent the fluid motion, this aspect must be dealt with separately. Each of these effects occurs in length scales ranging from the largest in the domain to the smallest; therefore, the inertial contribution operates within length and time scales that are most likely different from the other two terms. Diffusion is inherently seen as a molecular process so it is considered to be within the range of the
Kolmogorov scale and smaller. Likewise, the chemical source terms are at or below the scale of the diffusion process. Regardless of whether these processes are fast or slow, they occur within a molecular scale, which is generally the smallest considered in most studies. Due to the drastic length and time scale differences between the advection terms and the molecular processes, a supposition can be made that the terms can be linearly separated in a time-marching numerical algorithm without any significant losses (Kerstein A., 1999). This step in the analysis is important because once the conservation equations are converted to a 1-D representation, the advection terms are no longer mathematically consistent with the rest of the equations.

In order to reduce the conservation equations down to a single dimension, two additional assumptions must be added. First, the conservation of mass must be converted to an equation of state so the fluid has to be assumed to follow the characteristics of a perfect gas. Next the viscous forces in Eq. (2.5) are assumed to be dependent only on shear stresses.

\[
\frac{\partial \tau_{xy}}{\partial y} = \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) \tag{3.7}
\]

Equations (3.2), (3.3) and (3.5) can be reduced to one dimension by replacing the advection term with a function having an equivalent effect stochastically.

\[
\frac{\partial u}{\partial t} = \Omega(u, y) + \frac{1}{\rho} \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) - \frac{1}{\rho} \frac{\partial P}{\partial y} \tag{3.8}
\]

\[
\frac{\partial T}{\partial t} = \Omega(T, y) + \frac{1}{\rho c_p} \left[ \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) - \rho \left( \sum c_{pk} Y_k V_{yk} \right) \frac{\partial T}{\partial y} \right] - \omega_T \tag{3.9}
\]

\[
\frac{\partial Y_k}{\partial t} = \Omega(T, y) + \frac{1}{\rho} \left[ \frac{\partial}{\partial y} \left( \rho Y_k V_{yk} \right) + \omega_k \right] \tag{3.10}
\]
The function $\Omega(\phi, y)$ is the stochastic function for advection. It provides the replacement for the non-linear advection within a domain of reduced dimensions. $\Omega(\phi, y)$ operates on a different time scale than the diffusion and reaction contributions, so it must be implemented such that the time-marching algorithm can alternate from advection to diffusion and reaction during each time step.

A key aspect of ODT is the ability to reduce problems with dominant downstream motion to first a two-dimensional domain having the downstream position determined by the fluid velocity taken during a given time window (Kerstein A., 1992). For problems involving planar or axial jets, which are considered axisymmetric, the domain can further be reduced down to one dimension. What remains is a single line in the transverse direction across the interface boundaries. The state of this domain at a given time is a snapshot of the flow at the position corresponding to where the bulk velocity would carry the mixture during the last time interval. In the transverse direction, the remaining effects of advection are the turbulent stirring and entrainment of fluid from the boundaries. Turbulent stirring is the mechanism by which energy is transferred within the inertial sub-range, and entrainment is the result of advection working with the boundaries conditions. Stirring is also responsible for permutations within each fluid element resulting in the bulk mixing of constituent species. Molecular mixing is left to the deterministic diffusion processes, but bulk mixing provides a significant contribution to the fluid motion within a turbulent flow.

### 3.3 ODT and LEM Maps

The stochastic model designed to illustrate advection is a random selection of events which cause a functional permutation based on a randomly selected size. This process is
governed by an eddy rate distribution which determines the possibility of a change in the fluid. This rate is a function of Reynolds number and the velocity gradient in the transverse direction which are reflective of the amount of energy present. Event selection is sequenced within the time iteration loop using a probability based on several input parameters and data within the solution. These events render a decision whether an event can occur at a particular time. Similarly, the eddy size and location are determined based on the domain description and captured statistics. The functional permutation required for stirring is one where the scalars and velocity components are mutated within the locale of the selected eddy size. Ideally the function should be conservative and provide continuity at the boundaries of the target eddy.

As discussed in the original LEM formulation, a simple yet appropriate selection for the permutation function is the triplet map. The triplet map provides a 3x compression, as well as a flip operation, rendering the mixing result. In a functional sense the map is a 2 step process where the data is first compressed by one third in length scale, and then the middle region is reversed. The effects of this operation on a linear quantity are illustrated in Figure 3.1, which shows the compression and turnover effects on a simple function. The compression step performs the length scale reduction expected from the eddy cascade within the inertial range of turbulence, and the reversal of the middle region executes the necessary stirring to provide turbulent mixing. There are a few other things to note about the triplet map. First, it is piecewise continuous, not allowing for any discontinuities or singularities. Second, if the region within the eddy is considered a control volume, the external view is conservative such that the boundaries are unchanged. Finally, because the triplet map is essentially a function applied to a data signal, reapplication of the function renders signals of smaller and smaller wavelengths achieving the necessary wave number reduction (or energy cascade).
The functional form of the triplet map appears as a shuffling of data within a mapped region. The data points are not modified, only duplicated and rearranged.

\[ \xi(y, l, y_0) \tilde{\psi} = \xi(\tilde{\psi}(y, l, y_0)) \]

\[ \tilde{\psi}(y, l, y_0) = \tilde{\psi} \left[ y_0 + \begin{cases} 
3(y - y_0); y_0 \leq y \leq y_0 + \frac{l}{3} \\
2l - 3(y - y_0); y_0 + \frac{l}{3} \leq y \leq y_0 + \frac{2l}{3} \\
3(y - y_0) - 2l; y_0 + \frac{2l}{3} \leq y \leq y_0 + l \\
y - y_0; \text{otherwise}
\end{cases} \right] \]  

(3.11)

The eddy location is defined by \( y_0 \) and the eddy size being determined by \( l \). The mapping events are then articulated as a function of \( \tilde{\psi}(y), y_0 \) and \( l \).

\[ \Omega(\xi, y) = \xi(y, l, y_0) \tilde{\psi} \]

These event functions are the stochastic replacements for the advection terms in the transport equations.

\[ u \frac{\partial u}{\partial y} \cong \Omega(u, y) \]  

(3.12)

\[ u \frac{\partial T}{\partial y} \cong \Omega(T, y) \]  

(3.13)

\[ u \frac{\partial Y_k}{\partial y} \cong \Omega(Y_k, y) \]  

(3.14)
While not explicitly stated, it is important to note that during the stirring time step, the density is mixed along with the other solution variables, while during the reaction-diffusion step it is updated using the perfect gas equation of state.

![Triplet Map transformation](image)

**Figure 3.1** Triplet Map transformation

### 3.4 Eddy Selection

During each time iteration several factors determine when and where an eddy event occurs. The occurrence of mapping events is determined by an eddy rate distribution. The eddy rate distribution is inversely proportional to a length squared and the characteristic local time scale.

\[
\lambda(u, y_0, l) = \frac{1}{l^2 \tau(u, y_0, l)}
\]  

(3.15)

The length \(l\) is determined by the eddy size, and \(\tau\) is the associated timescale. Because eddies are driven by velocity gradients, the local time scale can be defined as a function of the local velocity gradient and the fluid viscosity.

\[
\frac{1}{\tau} = \sqrt{\left[\frac{A(U_L - U_R)}{l^2}\right]^2 - \left(\frac{16\hat{\nu}}{l^2}\right)^2}
\]  

(3.16)
\( \hat{\nu} \) is the characteristic viscosity associated with the eddy of size \( l \). As is evident in Eq. (3.16), the term on the right hand side under the radical must be positive in order for an eddy to be physically possible. Having a positive value here means that there is enough shear energy to overcome the viscous dissipation. Other cases where the characteristic time is greater than the solution time are also not possible, thus they, too, must be prohibited. The free parameter \( A \) provides tenability to how much shear energy is required to generate an eddy event. In general, the simulation procedure first samples an event based on a calculated time step, and then using the above equations to determine if the event is possible. If the events are sampled too frequently, the model performance suffers. If the events are not sampled frequently enough, then the events won’t match the physical characteristics of the problem. Thus, a method is needed to determine accurately an effective time step driving the events. A simple method based on the pdfs of \( y_0 \) and \( l \) was devised early on by Echekki et. al. which has proven to be quite useful (Echekki T., Kerstein, Dreeben, & Chen, 2001).

\[
\lambda(t, y_0, l) \Delta t_s = P(t, y_0, l, \Delta t_s) f(l) g(y_0) \tag{3.17}
\]

With this implementation, the eddy size and location is selected randomly based on the distribution, and the time step is validated via the probability \( P \). The maximum probability from the above calculation is combined with a prescribed probability target to scale the time step, allowing for unlikely events to be excluded. During each ODT time iteration, Eqs. (3.8), (3.9), and (3.10) are solved separately through a gated selection, activating either the advective stirring equations (left) or the reaction-diffusion equation (right). The gate is determined by the alignment of the current time step with a preset range of associated time steps (Cao S., 2006). In Figure 3.2, the reaction-diffusion ranges (\( \Delta t_{CD} \)) are represented by the hash marks above the line, and the advective ranges (\( \Delta t_\Omega \)) are represented by the hash
marks below the line. As the solution progresses, the time step that falls next in the progression is selected and the corresponding equations are solved. As both time steps ($\Delta t_{CD}$ and $\Delta t_{\Omega}$) are calculated from solution variables, the amount of time until an equation is solved varies.

**Figure 3.2** ODT Time steps

With the key time steps defined as $\Delta t_{CD}$ and $\Delta t_{\Omega}$ the ODT time-marching algorithm can be expressed in a single equation.

$$
\Phi^{n+1} = \Phi^n + \Delta t_{CD}(1 - \delta_\lambda)R_{CD} + \Delta t_{\Omega}\delta_\lambda\Omega(\Phi^n) 
$$

(3.18)

$\Delta t_{\Omega}$ is governed by the model parameters and the probability from the expression for $\Delta t_z$, and $\Delta t_{CD}$ determined by stability limits due reactive-diffusive equations. Statistics are collected on a much larger fixed timescale and don’t play into Eq. (3.18). Each time step is updated during the time loop and the next active process is determined by which time step is closer to the calculated time values falling after the previous iteration is complete. $R_{CD}$ is the RHS of the reactive-diffusive equation and $\Omega(\Phi^n)$ is the operation resulting from the triplet map.
Finally, $\delta_\lambda$ is the gate determining if an advection event is allowed during the current iteration. Included in Figure 3.2, convection is the target time for advancing the solution downstream.

Albeit simple, reducing the non-linear convolution $\frac{\partial \rho u_i u_j}{\partial x_j}$ down to a stochastically determined linear effect allows for a very efficient solution method in one dimension.

### 3.5 Source Terms

Having the turbulent stirring and the molecular processes separated, time advancement of the equations containing the $R_{CD}$ terms can be as complex as necessary to capture the desired degree of combustion complexity. In addition, having the solution linearly separated also enables implementations that use innovative methods that facilitate highly detailed reaction mechanisms. In particular, solutions for complex chemistry must account for a stiff set of ODEs because of the large differences in time scales of each rate contribution within the reaction mechanism. Alternative methods aside, a typical direct solver for a multi-step reaction mechanism uses a method based on law of mass action with Arrhenius rate calculations (Kuo, 2005). Applying this concept, the source term for each of the species equations is the sum of the rate changes which are calculated from each of the included reactions.

$$\omega_k = \sum_{i=1}^{N} (v_{ki}'' - v_{ki}') R_i$$  \hspace{1cm} (3.19)

$R_i$ is the rate of change for reaction $i$ and $(v_{ki}'' - v_{ki}')$ is the difference between the product and reactant coefficients for species $k$ in reaction $i$. The change rate for a reaction is measured from the species concentrations weighted by associated reaction rates.
\[ R_i = k_{fi} \prod_{k=1}^{K} (C_k)^{v_{ki}} - k_{bi} \prod_{k=1}^{K} (C_k)^{v'_{ki}} \]  

(3.20)

Now the forward reaction rates are defined with a temperature dependence based on the Arrhenius rate equation.

\[ k_{fi} = A_i T^{\beta_i} \exp \left( -\frac{E_{ai}}{R_u T} \right) \]  

(3.21)

A_i, \beta_i and \( E_{ai} \) are constants unique for each reaction. \( E_{ai} \) represents the amount of energy needed to overcome a particular reaction to proceed, and \( A_i T^{\beta_i} \) captures the reactive state of the molecules. The backward rate is defined as a function of the forward rate and an equilibrium constant.

\[ k_{bi} = \frac{k_{fi}}{k_{ci}} \]  

(3.22)

The equilibrium constant is a function of the pressure, temperature and other reaction specific values such as entropy and heat of formation.

The source term for the conservation of energy equation is a function of each of the source terms for the species equations weighted by the amount of energy potential contained within the molecule.

\[ \omega = \sum_{k=1}^{K} h_k^{\theta} \omega_k \]  

(3.23)

The energy source term is thus a function of the temperature and the mass fractions of each of the constituent species which have a RHS dependency on each of the species as well as the temperature. To illustrate this point, Eqs. (3.9) and (3.10) can be written in vector form showing the dependency included within each function.
\[
\frac{\partial \vec{U}}{\partial t} = D(\rho, T, Y_k) + \vec{R}(\rho, T, Y_k)
\]  

(3.24)

Depending on the complexity of the reaction mechanism, integrating eq. (3.24) may require either an implicit or semi-implicit technique to account for equation stiffness. An implicit integration requires linearizing the RHS term \(\vec{R}^{n+1}\) which is the RHS for the next time step.

\[
\vec{R}^{n+1} = \vec{R}^n + \frac{\partial \vec{R}}{\partial \vec{U}} (\vec{U}^{n+1} - \vec{U}^n)
\]  

(3.25)

Equation (3.25) presents a significant challenge because the term \(\frac{\partial \vec{R}}{\partial \vec{U}}\) is a matrix that includes many elements that differ by several orders of magnitude.

A simple yet robust method which properly handles this problem is a 2nd order Runge-Kutta method where the first iteration uses an explicit application calculating the RHS from a CHEMKIN formulation of the chemical reaction. The interim solution vector is then used to estimate \(\frac{\partial \vec{R}}{\partial \vec{U}}\) in the VODE solver, ultimately determining the final solution vector. The CHEMKIN routines are based on the previously public domain CHEMKIN II version, and the VODE solver is both found in the ODEPACK, which is available through the Lawrence Livermore National Laboratory (Hindmarsh, 1983).

### 3.6 Reduction of Dimensionality

While ODT is intended to reduce the computational environment to a single dimension, the problem to be solved remains within a three-dimensional space. As a result, ODT must provide a mechanism to relate results back to the original problem domain. Because the flow within an ODT domain is developed temporally, the downstream distance can be represented
using the bulk velocity and the instantaneous time. Over time, a picture of the simulated 3D domain is implied by the collective results of each iteration. This enables collection and analysis of a variety of important pieces of information. As a stand-alone simulation, the data collected from each iteration can be assembled to show a 2D result. For symmetric problems this view is sufficient, but for cases where symmetry is not warranted, additional ODT domains must be combined to illustrate the entire domain. For the problems in this study, an axisymmetric ODT solution is sufficient. Along with the 2D view of the solution, researchers can also gather statistics needed to analyze and construct data distributions. This data can be collected over time at a given location, or it can be collected as an ensemble. Either way, having the data in either the spatial domain or state-space provides valuable information concerning the flow.

3.7 Parameter Selection

Even though ODT provides a decent reduction in the empiricism previously required for similar solutions based exclusively on LEM, several model parameters are still necessary to produce valid solutions for target domains. As mentioned in the original research outlining the use of ODT, the two most important parameters are the free parameters $A$ and $\beta$ (Kerstein A. , 1999). $A$ is a scaling factor that helps determine how much strain is necessary to overcome the viscous dissipation, thus causing an eddy event. The strain field is an essential component within a turbulent flow because it provides the driving layer in which turbulent energy is transformed into eddy motion. This parameter, $A$, is the link between the strain field seen in a particular problem domain and the fluid mix selected. This parameter is of the order of unity but must be scaled accordingly. For most problems involving shear layers (channels or jets)
this parameter is set to 0.3. $\beta$ determines the reaching effects of the turbulent flow. This value for most part controls how much the turbulent field grows over time. It provides a threshold for turbulent growth. In addition to $A$ and $\beta$, parameters are necessary to give variability to the time selection procedure as well as limiting eddy selection. The time selection parameter is in the form of a target probability. This parameter, combined with the calculated probability, forms a ratio scaling the next time step needed for advection. It should be in the order of the calculated probability so that the scaling is reasonable. Finally, to prevent unnecessary or unrealistic eddies, two parameters are added to limit the minimum and maximum eddy sizes accordingly.
4 Kernel Density Function and LES Closure Construction

4.1 Introduction

When experimental flames are studied to determine the effects of turbulence in non-premixed flames, important information is gained from analyzing conditional mass fractions and their corresponding distributions. For the most part each of these distributions demonstrate a single modal shape for flames containing lower levels of turbulence, but become more spread out and eventually splitting as the turbulence increases. (Barlow & Frank, 1998; Barlow R., 1999) show that in Flames A-D each of the species studied mainly exhibited distributions with only a single mode. In contrast, Flame F and in some cases, Flame E produced shapes with two or more modes in regions having higher variance levels. Figure 4.2 illustrates this trend for the conditional PDF of H$_2$O mass fraction. At $x/d=15$ and to a small degree at $x/d=30$, the PDF for Flame F shows a departure from the PDFs for Flame D and Flame E. The conditional PDF for $Y_{H_2O}$ in Flame F distinctly exhibits a bimodal shape at $x/d=15$ which is shown to link directly with flame instabilities. Similar trends are also observable in the conditional PDF for temperature as seen in Figure 4.1.

These observations highlight the importance of using distributions that more accurately reflect the nature of the flame when integrating an LES closure function to predict filtered source terms in highly turbulent flames. As has stated previously, single modal distributions such as the $\beta$-PDF are best used with flames that are known to contain minimal extinction effects. This choice is appropriate when comparing the curves for Flame A-D in Figure 4.2 to Figure 4.3 with the sample $\beta$-PDF curves in Figure 4.5. In Flames A-D the conditional PDFs collapse into a single modal distribution much like the $\beta$-PDF; however, in Flames E
and F, the shapes of the PDFs are not consistent with the $\beta$-PDF. A better solution then, is to use PDFs that better reflect the nature of the turbulent flame. In contrast to LES closure using $\beta$-PDF, the ODT-LES closure model captures these turbulent effects by including simulated distributions that better reflect the nature of the flames. As the PDFs are believed to be the result of scalar mixing and turbulent fluctuations, ODT provides the basis for equivalent distributions by stochastically and numerically modeling the interaction of these processes.

The challenge then is to extract these distributions from the results of an ensemble of ODT realizations, and to formulate a functional equivalent that is useable in a numerical integration of the PDF with scalar statistics. The Kernel Density Estimator is an excellent method to functionally represent the statistically generated distribution which is needed for LES closure of a turbulent flame. Applying a KDE to distribution samples produces a numerical PDF that has similar mathematical properties to the $\beta$-PDF while also better capturing the nature of the turbulent flame. The remaining sections of Chapter 4 describe the process by which ODT realizations are used to gather the statistics and construct the numerical distributions needed for LES closure.
**Figure 4.1** Conditional PDF of temperature for Sandia Flame D, E, & F from experimental results (Barlow R., 1999)

**Figure 4.2** Conditional PDF of $Y_{H_2O}$ for Sandia Flame D, E, & F from experimental results (Barlow R., 1999)
Figure 4.3 Conditional PDF of $Y_{OH}$ for Sandia Flame D, E, & F from experimental results (Barlow R., 1999)

Figure 4.4 Conditional PDF of $Y_{CO}$ for Sandia Flame D, E, & F from experimental results (Barlow R., 1999)
Sample $\beta$ – PDF Distribution

Figure 4.5 $\beta$-PDF Sample Distributions
4.2 Model Definition

The LES solution for the piloted non-premixed turbulent jet flame is closed using a table defined within the filtered state-space which provides filtered values for the fluid density, the chemical source terms, and the source term appearing in the temperature variance equation. The lookup terms for this closure table are the filtered state variables -- mixture fraction and temperature -- along with the scalar variances, but the input needed to construct the table originates in the ODT domain, which is spatially resolved. The construction process requires a correlated set of filtered and unfiltered (spatially resolved) vectors in state-space, which is organized to provide conditional statistics as well as distribution information. The final lookup table is the discretized result of performing the integration defined by Eq. (2.42) which requires FDFs for each state variable and conditional statistics for each of the dependent variables. The conditional statistics needed in this integration come from ensembles collected via realizations of an ODT simulation configured to match the sample domain. Likewise, the integrated distributions are constructed with a similar set of data which correlates filtered and unfiltered stated variables falling into select ranges of the scalar variance. The filtered state variables and the variance values are independent inputs to the construction algorithm, and thus they are also the conditioning variables used to manage the raw statistics. The variance lookup values are aligned with the selected the FDF needed in the integration, and they are selected based on ranges which provide the best coverage of the overall solution. The remaining sections in this chapter cover the collection and processing of the data needed in the integrations, the distribution construction using KDE, and the integration of the final closure table.
4.3 Model Construction

Model construction is a multi-step process that starts with running a set of ODT simulations that have the same initial conditions differing only in the seed data for generating randomness. From these ODT realizations, sets of one and two-dimensional data are organized by mixture fraction, temperature and the ODT determined variance. The ODT determined variance is calculated from Eq. (2.44) using known quantities in the ODT domain. In order for the raw data to be useful, it must go through several preprocessing steps to eliminate redundancy, fill in gaps where data has not or cannot be captured, and to remove noise resulting from statistical outliers. Correlated vectors containing resolved (unfiltered) state variables with their first and second moments are needed to build the filter density functions. The random datasets are reorganized as sample counts for given first and second moments which are in turn inputs into parametric distributions using a kernel density estimator. The conditional statistics also go through several different steps to eliminate noise and completely fill in the table with smooth data. Once all the preprocessing is completed, the final step applies the FDFs with the statistical data performing the filtering integration. The resulting 4D table contains filtered dependent variables that are needed for LES closure of conservation equations as well as a selective set of mass fractions that are applied during post processing to illustrate the chemical state of the system.

The construction process is illustrated in Figure 4.6 where the applications are the numbered boxes and the artifacts are lettered boxes. The ODT simulation (1) is a modified form of the Fortran code used by (Echekki T., Kerstein, Dreeben, & Chen, 2001) to model extinction and re-ignition. This code saves ODT data in an ensemble of correlated vectors (A) which contain all the necessary information for LES closure. The Pre-processing step (2) is a
custom Fortran code used to split the un-order solution vectors into a 2D table (B) of conditional statistics in state-space and an un-ordered set of distribution samples (C) required for FDF construction. The post processing steps are executed with a set of custom utilities written in C++ and Matlab. The post processing step (3a) on the conditional statistics table finalizes the interpolation process, providing a complete representation of the conditional statistics for all possible combinations of the state variables. The post processing step (3b) on the distribution data first prepares the data for sorting, then it organizes the distribution vectors by variances and, finally, the set of Matlab scripts perform the FDF construction via kernel density functions. The last step (4) is the integration application (C++) which takes the finalized 2D table (D) of conditional statistics and the generated FDF table (E) and performs the filtering integration over the target state-space. The final artifact (F) is a 4D table which contains $3+k$ values including the density, the chemical source term, the temperature variance source term and closure for $k$ species mass fractions.
Even though turbulent scalars are expected to be random, attempting to predict these quantities with a distribution function containing noise can be challenging. Numerical solutions have strict constraints limiting the error growth, and thus a noisy distribution introduces unwanted numerical errors, which may impact the solution negatively. To prevent this issue, a method to learn a smooth representation of the distributions found in ODT solutions must be considered. The Kernel Density Function (KDF) is a continuous representation of a distribution function based on input samples, which may contain sparse
data as those seen with actual data. A KDF is expressed as a sum of kernel functions centered on model determined points, which are learned from the sample data (Bowman, 1997).

\[
P(x) = \frac{1}{nh} \sum_{i=1}^{n} K \left( \frac{x - X_i}{h} \right)_{\text{4.1}}
\]

\(K\) is a prescribed single mode continuous density function, \(n\) is the number of sample points, \(X_i\) are the samples, and \(h\) is the bandwidth for each kernel. The degree to which a kernel function can model a given dataset is determined by the bandwidth and the number of samples provided to the estimator. Thus, the keys to learning such a function are determining the best choice for the sample size and selecting the necessary bandwidth. Larger bandwidths generate smoother functions while the smaller bandwidth proves to be more accurate. Too many samples with a small bandwidth generate curves more closely matching the samples, but this locally varying data may not work best with a filtering integration. In contrast, too few samples with a larger bandwidth generate curves that are less likely to capture all of the trends present in the distribution. These parameters must be balanced and appropriate for each implementation. The number of samples and the bandwidth can be pre-defined or determined through different estimation techniques (Martinez & Cho, 2015).

Extensions to the KDF method define each kernel with weighting coefficients in order to balance the bias based on important features in the distribution.

\[
P(x) = \sum_{i=1}^{n} \alpha_i K \left( \frac{x - X_i}{h_i} \right)_{\text{4.2}}
\]

This technique is much more accurate, but it does require a more complex learning process with more parameters to manage. The additional weighting factors are learned by solving the
minimization problem resulting from evaluation of the moments with the given distribution samples (Athanassoulis & Gavriliadis, 2002).

\[
\left\| \mu_n - \sum_{i=1}^{I} \alpha_i x^n K(X_i) \right\|_{L^2} = \min ; n = 0, 1, 2, ...
\]  

(4.3)

\( \mu_n \) are the moments found in the test data and \( \alpha_i \) are coefficients to be determined.

An implementation of learning and representing distributions via kernel density estimators exists within the Matlab statistics toolkit. Appendix B describes in detail the content of scripts designed to invoke these routines, and subsequently generate the distribution tables needed for integrating filtered quantities. The sample set originates from ODT observations, and the final results are stored as normalized distributions ready for table integration. The Matlab toolkit expects data organized as sample counts, but the ODT observations are random samples. In response, the process to construct a kernel density function representing ODT distributions is a multi-step process where the ODT samples are first reorganized as counts followed by a distribution training step.

### 4.5 FDF Construction using Kernel Density Function

A precursor to organizing the ODT distribution samples applied in the KDF learning process is representing the distributions in the form of a histogram. Covered in more detail in Appendix D2, a histogram distribution is a discrete function which represents a dataset through a set of normalized sums. With variance being one of the independent variables, the histogram collections that represent ODT distributions include variance as one of the dimensions. The ODT datasets are assembled using these ranges in order to construct a histogram distribution that matches the discrete variance ranges. Following the constraints outlined by (Cook &
Riley, 1994), the filtered variance is determined within the ODT domain from filtering the independent scalar and its square.

\[ \Phi \tilde{\Phi} = \Phi^2 - \tilde{\Phi}^2 \]  

(4.4)

With this definition, the variance can be included in the correlated vectors that make up the ODT distribution dataset. A mathematical description of the histogram distribution vectors can be articulated within the ODT domain using the resolved and filtered variables along with the variance.

\[
P(\varphi_j, \varphi_k, \varphi_l) = \frac{1}{n} \sum_{i=1}^{n} \begin{cases} 
1 & \varphi_j \leq \Phi_i < \varphi_{j+1}; \\
\varphi_k \leq \Phi_i < \varphi_{k+1}; \\
\varphi_l \leq \Phi_i \Phi_i < \varphi_{l+1}\varphi_{l+1} & \varphi_j > \Phi_i; \Phi_i \geq \varphi_{j+1}; \\
0 & \varphi_k > \Phi_i; \varphi_i \geq \varphi_{k+1} \\
\varphi_l \geq \Phi_i \Phi_i; \varphi_i \geq \varphi_{l+1} \varphi_{l+1} \\
\end{cases}
\]  

(4.5)

Using Eq. (4.5), histogram distributions sorted by variance are constructed from the unordered ODT data sets according to the discrete variance. The histograms provide the samples needed to “learn” the FDFs via a kernel density function, but building the density functions works best when the histograms have more complete datasets. Interpolation and smoothing are not necessary because the kernel density functions inherently smooth the data; however, the sample data provided to the density estimator must be in a format that provides a good set of data points for each data range. The sample data is organized as counts of data points that lie a discrete distance from the tabulated mean. These sample counts are normalized so that the KDE fitting routine operates consistently regardless of the amount of data available. For sample sets that are not complete additional work is done to prepare the sample set. Depending on the amount of data available, either data from surrounding distributions are combined with
what data is available or a default curve is supplied. These cases are rare and tend to lie outside the expected range of realistic data, but must be included for the process to operate properly. In general the default sample is a simple Gaussian curve which distributes the data points evenly, but if the data is too sparse the $\beta$-PDF is a better choice.

The collection process for FDF histograms considers the non-linear nature of the available data samples. Following the operation described in Eq. (4.5) the filter density functions are organized using discrete buckets representing the associated variance range. A typical normalization algorithm assumes that the normalized values are distributed evenly; however, in cases where the normalized values span multiple orders of magnitude, normalization overemphasizes the data elements in the upper regions making little use of the mid region of the data. Figure 4.7 illustrates the large differences in magnitude for each of the scalar variances collected from an ODT simulation. In both plots, more than three fourths of the data fall in a range that appears negligible, yet these collections are a good portion of what must be considered. The scalar variance maps to reference indices in the closure table without any reconstruction, and thus the strategy applied to deal with the scalar variances need only be concerned with categorization. The only question that needs to be answered is where a sample belongs based on the scalar variance.
A straight normalization based on such a large span of magnitudes places the bulk of the data into a small portion of the normalization range. To alleviate these issues, the criteria with which to select the discrete variance values first is simplified by taking the $\log_{10}$ of the variance. The normalization procedure is then applied to the result. A few issues must be noted with this approach before continuing. First, the logarithm of zero is undefined, so as the variance approaches zero, the value becomes more negative until it is no longer valid. Keeping in mind that the objective is to divide the variances as evenly as possible, the $\log_{10}$ result for zero is arbitrarily defined as a large negative number. Also, even though the $\log_{10}$ operation brings the discretized values closer together, the values still exhibit an asymptotic character at the ends. Thus, in addition to arbitrarily setting the value for zero, boundaries are selected to best ensure an evenly distributed set of ranges. The first range includes the zero value up to the lower boundary, and the last range includes the upper boundary and beyond to the largest available sample. This added step simplifies the organization of the FDF samples and makes table construction more feasible. Figure 4.7 shows the $\log_{10}$ of the scalar variances along with

**Figure 4.7** Scalar Variance collections for Flame F

![Figure 4.7](image-url)
a linear curve fit approximation. With the curve fit graphed, the upper and lower bounds for categorization can be best determined as the points where the lines intersect. These data boundaries are, then, part of building the histogram datasets, which are the training source for the kernel density function.

\[
\text{Log}_{10} \text{ Variance Curve Fit — Flame F}
\]

**Figure 4.8** Curve fit of \( \text{Log}_{10}(Z''Z'') \) and \( \text{Log}_{10}(T''T'') \)

The key factor when selecting the boundaries above is uniformity of distributions for each of the discrete data ranges within the overall dataset. If too many sets end up in a smaller number of ranges, then the distributions won’t be as representative as desired. The result is cross checked by evaluating the width of each distribution which is representative of the discrete variance. If the widths aren’t appropriate for each of the variance labels then the boundaries are re-evaluated. There are three factors that must be considered. First, the number of discrete ranges for the collection of variances. The number of ranges affect the amount of data available for each distribution sample set, but it also has an effect on the size of the closure table. Considering that the size of the closure table is already compounded because there are four variables included in the lookup, adding one additional bucket to the number of discrete
variances doubles the table size. After determining the number of discrete ranges that are possible, the total width of the log variance data is considered. This width determines the individual widths of each range, and thus the selection should allow for a decent number of choices in each range. Finally, the positional placement within the available data values must be chosen. The boundaries selected for categorizing variance values have a large impact on the final distribution in that it determines the model’s ability to capture the highly divergent values effectively.

The FDF table is constructed using a four step process. These processes are a combination of manual selections as well as automated numerical routines. While the process by which the ranges are selected could be automated, such an effort is beyond the scope of this research and should be considered elsewhere. Each individual step is outlined in Table 4.1. The data file resulting from step 4 is essentially VxN distributions, where V is the number of discrete variance ranges and N is the discrete number of filtered values.

Table 4.1  FDF Construction Process

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
<th>Implementation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Evaluate the datasets and select appropriate discrete boundaries</td>
<td>Manual selection from graphical data</td>
</tr>
<tr>
<td>2</td>
<td>Using the boundaries to determine the data range for each variance and the associated limits, collect samples from the available data and create histogram datasets based on instance counts within an appropriate standard deviation</td>
<td>Automated C++ program</td>
</tr>
<tr>
<td>3</td>
<td>With the histogram datasets, construct input files needed to build distributions using kernel density estimator.</td>
<td>Automated MATLAB script</td>
</tr>
<tr>
<td>4</td>
<td>Build distributions using the kernel density estimator and save results in a 3D table indexed by discrete variance, filtered value, and instantaneous value.</td>
<td>Automated MATLAB script</td>
</tr>
</tbody>
</table>
4.6 Pre-Processing Raw ODT data

As stated above, the data collections that result from the net sum of all the ODT realizations provide a decent view of the underlying patterns, but for mathematical reasons, performing the integration from Eq. (2.41) requires a more complete view of the state-space. For this reason, the information provided must undergo an interpolation process to fill in the gaps and the white space outside realistic state values must be populated. This white space is the open region between the flame and the outer boundaries in the state-space, and it must be filled in with data that best matches based on boundary conditions. Once these empty areas are filled, a 2D interpolation process can connect the regions, but the fields are only consistent if the outer boundary of the ODT flame data is contiguous. The first step in the interpolation process is to complete the outline around the given scatter data with known values that are consistent with the given samples. With the boundaries set on the outer regions of the state-space and the inner region surrounding the ODT samples, the white space is filled with gradients consistent for that area.

The phases of this construction start first with the assembly of the raw ODT samples, then the known boundary values are added, followed by interpolating the data comprising the outer edge of the raw ODT samples. The outline around the ODT sample region is determined using 1D spline, connecting the points between different samples along the outer portions of the dataset. The outer portions of the state-space boundary are determined by a combination of non-reacting ODT realizations and prescribed values based on the problem definition. Empty regions where all the samples are not complete are intentionally left out to be filled in with the final interpolation step. With the approach, the areas leading up to the core regions are filled with continuous data that is consistent with known values.
4.7 Post-Processing Raw ODT data

The data from aggregated ODT realizations cannot account for every possible location, and thus it is necessary to fill the gaps with an appropriate interpolation routine. For years, multivariate interpolation has been used for image processing, resampling and scaling as well as many other data matching algorithms (Kreyszig, 2011). In fact, (Cao S., 2006) uses a multivariate linear interpolation to scale data in the ODT domain to match the velocity field in the LES domain. The basic idea behind multivariate interpolation is to fill in the missing data by using values from data locations that do contain values. The values pulled from each of the contributing known locations are weighted based on proximity to the calculated location. In a bilinear interpolation, the function for determining the interpolated data points uses the distances between the target location and the other four known locations. This formula gives more weight to the points closest to the target with the ratio of the surface area opposite source point to the surface area encased by all four points. While it is possible to perform these calculation with custom routines, when available, known working functions are the best option.

\[
v_{i,j} = \frac{x - x_1}{x_2 - x_1} \frac{y - y_1}{y_2 - y_1} v_{i+1,j+1} + \frac{x - x_1}{x_2 - x_1} \frac{y_2 - y}{y_2 - y_1} v_{i+1,j} + \frac{x_2 - x}{x_2 - x_1} \frac{y - y_1}{y_2 - y_1} v_{i,j+1} + \frac{x_2 - x}{x_2 - x_1} \frac{y_2 - y}{y_2 - y_1} v_{i,j}
\]

(4.6)

Matlab has developed a very successful set of interpolation routines which are used for interpolating the raw ODT data. The advantage this provides is the reassurance that the routines calculate values as expected, in an efficient manner. Once the interpolation is complete, a final smoothing step is applied to the 2D table to ensure that noise generating artifacts don’t produce too much error when the integration algorithm is executed. The smoothing step is a simple diffusion routine which models the 2D heat equation.
\[ \frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \] (4.7)

The heat equation has been shown to produce the necessary results of eliminating regions with artificially produced gradient; however, it must be applied carefully and in a limited fashion. Too much smoothing with iterations that are too large can effectively smooth out the image into a constant value (Kimia & Siddiqi, 1996). Each iteration using Eq. (4.7) has the effect of removing information from the given dataset. Removing too much information leads to a more RANS like collection, where the final image is simply a smear. Thus, the diffusion step is performed with a very small time step and a limited number of iterations so as to minimize the amount of information lost. While this process does carry a degree of loss, it is necessary that the final table be free of discontinuities and unnatural fluctuations.

### 4.8 Final Integration

The final integration combines the FDF distributions with the complete table of ODT solution data. Normalizing the state variables before integrating simplifies the lookup process and makes the integration procedure symmetric. As mentioned above, the variance values are already normalized in order to ensure evenly distributed values. The mean (filtered) values require a similar type of normalization, as well as the instantaneous values stored in the raw datasets. While no arbitrary boundaries are required to ensure that the ranges aren’t skewed, the normalization method is equivalent: normalize the state variables, followed by dividing the domain into equally sized parts. With equally sized parts, the Trapezoid rule can be applied making the integration a simple arithmetic operation.
\[
\int_{x_0}^{x_n} f(x) \, dx = \frac{\Delta x}{2} \left[ f_0 + 2f_1 + 2f_2 + 2f_3 \cdots 2f_{n-1} + f_n \right] \quad (4.8)
\]

This procedure works best for datasets where the majority of the values are greater than unity. In cases where the values are less than unity, the combination of these values does not render the desired result. To best deal with this, the integration is performed over the inverse of a given value, and then the final result is the inverse of that term.

\[
\tilde{\rho} = \frac{1}{\iiint \frac{1}{\tilde{\rho}} P(Z, \tilde{Z} \cdot \tilde{Z}^n) P(T, \tilde{T} \cdot \tilde{T}^n) dT dZ} \quad (4.9)
\]

As seen in Eq. (4.9) this procedure is used to obtain the filtered density table. The filtered source term \( \left( T^\omega \omega_T \right) \) which show up in the temperature variance transport equation is obtained by the linear combination of \( \omega_T \) and \( \omega T \) according to Eq. (2.47). In this equation \( \omega \) is the filtered chemical source term and \( \tilde{T} \) is the filtered temperature which corresponds to the lookup value for that section of the table. Note that \( \omega \) is the same source term which is intended for inclusion in the closure table, so it is integrated prior to calculating \( \left( T^\omega \omega_T \right) \). The additional value that must be integrated to obtain \( T^\omega \omega_T \) is \( \omega T \).

\[
\omega T = \iiint T \omega(Z) P(Z, \tilde{Z} \cdot \tilde{Z}^n) P(T, \tilde{T} \cdot \tilde{T}^n) dT dZ \quad (4.10)
\]

The procedure is simple:

1. Loop through each of the discrete variances and filtered values for both temperature and variance
2. Within each loop perform the following integrations
   a. Integrate density using Eq. (4.9)
   b. Integrate temperature source
   c. Integrate \( \omega T \)
d. Calculate $T^\omega \omega_T$.

3. After integration loops are complete normalize the results

4. Save normalized table as 4D indexed binary data file. (Note that step 4 was added to make the table more portable allowing for adjustment based on scaling.)
5 Piloted Jet Diffusion Flames

5.1 Sandia Flames

The Sandia Flames are piloted jet diffusion flames executed at varying degrees of turbulence (Barlow R., 2016). Identified with letters A-F, the Sandia Flames range in intensity from transitional to fully turbulent, thus providing a good data collections to consistently measure flame characteristic and the varying effects of turbulence. The less intense C and D flames exhibit less finite rate chemistry effects; but they are useful for validating a model’s effectiveness in capturing the reaction-turbulence interaction. The flames with higher intensity E and F show finite rate chemistry effects, where extinction is more prevalent within in the highly strained regions. Re-ignition can also be seen in regions where the turbulent energy dwindles, leaving the reactions to proceed more to completion. For this reason, Flame F is often the focus of models intending to capture extinction/re-ignition effects in turbulent jet diffusion flames, while Flame D is used to evaluate the merits of proposed model changes.

When turbulence drives a diffusion flame to extinction, the condition is indicative of turbulent time scales that are smaller than the chemical residence time (IM, Law, Kim, & Williams, 1995; Meier, Barlow, Chen, & Chen, 2000). Modeling such a condition requires a good design that accounts for complex chemistry, without being restricted by global equilibrium conditions. A similar situation occurs in the states where re-ignition is triggered by relaxation in the turbulent intensity. As stated in the introduction, countless studies have been carried out with the goal of effectively capturing these conditions, using the resources available. To assist in this effort, several contributions to the Turbulent Non-premixed Flames (TNF) conferences have been experimental studies on the Sandia Flames (Barlow & Frank, 1998). The data
gathered in the initial studies and subsequent updates continue to be applied in computational comparisons to date, and thus the TNF Sandia Flame datasets are required to validate the computational results of the LES-ODT closure model. Appendix F provides additional background about the TNF organization, and their efforts to support turbulent combustion research.

5.2 Extinction and Re-ignition in Sandia Flames

Of all of the important features included with the piloted jet diffusion flame, the presence of local extinction and re-ignition are both of interest and value within the combustion research community (Barlow R., 2016). Non-premixed combustion occurs in the regions of the flow where fuel and oxidizer reach a stoichiometric mixture, and thus features that hinder this process are likely to also affect the flame. As the turbulent intensity is increased, the piloted jet diffusion flame provides this environment, where there is a balance between mixing which is positive to reaction progress and mixing that can hinder the reaction rates. (Barlow R., Frank, Karpetsis, & Chen, 2005) determined that while small amounts of extinction are observable in Flame D, regions showing local extinction become more prevalent in Flame E, and then even more so in Flame F. Analysis of the experimental data shows that the higher rates of mixture fraction decay correspond to regions of local extinction. This correlation would indicate that elevated mixing rates caused by the turbulence lead to extinction of the flame. In regions downstream, where the turbulence decreases, the rate of mixture fraction decay is slowed, allowing the chemistry to catch up with the reactants. Once they are caught up, the remaining reactants are permitted to ignite, leading to re-ignition. While other characteristics such as scalar dissipation and differential diffusion are noted in many of the
discussions, the general conclusions essentially reaffirm basic theories concerning these indicators. Scalar dissipation tends to be highest in regions where the velocity and scalar gradients are largest, and differential diffusion tends to play a more significant role where turbulent intensity stays under a certain limit (Sutherland, Smith, & Chen, 2005; Peters, 2000).

Ensuring that a computational model can capture local extinction is quite a challenge with many of the approaches used for non-premixed combustion. In general, the assumptions and mathematical theory applied to derive the model should be reinforced with the experimental analysis, but in the end the comparative results are what determine the effectiveness. Comparison of conditional values and their fluctuations provide a gauge by which to determine how well each model performs. Proceedings from TNF-4 note that the problem of predicting local extinction is quite difficult, and that because of the strong dependence on initial conditions, comparisons between models and experiments may lead to many more questions than answers (Barlow R., 1999). These proceedings also recognize that even with the same chemical reaction mechanism, different models predict different results in the near field fuel rich regions. While this may have something to do with the composition, as mentioned above, this near field fuel rich region $10 < x/d < 25$ corresponds to the area also showing more significant effects of local extinction in experimental flames. Later, in TNF-7, this correlation is established better with a comparison of how well a PDF transport model predicts local extinction with different mixing models (Barlow R., 2004). Needless to say, flame extinction is a very challenging problem not only to capture, but also to evaluate.

Each of the closure methods discussed in Chapter 1 have specialized studies which focus on predicting local extinction and re-ignition (Pitsch, Cha, & Fedotov, 2003; Kronenburg, 2004; Cao & Pope, 2005). For the most part, these studies use comparisons of
scalars conditioned on mixture fraction to determine the viability of the model. In contrast, (Cao, Wang, & Pope, 2007) adds an additional factor, labeled the burning index (BI), which is a relative measure of how well a mixture is burning. While this may be helpful, analysis of conditioned scalars and their fluctuations remain the key measurements of choice. Some studies use the temperature to determine local extinction, but others have used mass fractions such as OH, H₂ or CO, which would reflect the location of the burning flame (Sen, Hawkes, & Menon, 2010). These figures combined with analysis of scalar dissipation can assist in drawing a more complete conclusion of how well a model can represent extinction. This study focuses on conditioned scalars and spatial profiles of key species with RMS values to evaluate the effectiveness in capturing extinction and re-ignition.

5.3 Piloted Burner Configuration

The piloted non-premixed flame configuration consists of a round fuel jet surrounded by a round pilot burner, which is also surrounded by a coflow. The jet velocity is expected to operate at a much higher velocity than the pilot, which is also significantly larger than the coflow. For a CH₄/air burner configuration, the coflow is air, the fuel is CH₄ and air, and the pilot is equivalent to the stoichiometric mixture for CH₄ and air. Below is a list of the dimensions.

- Main jet diameter – 7.2 mm
- Pilot inner diameter – 7.7 mm
- Pilot outer diameter – 18.2 mm

The coflow velocity is the same for all flame configurations, but the fuel jet and pilot velocities are successively increased with flame label. For simplicity, the two flames of interest are
Flame D and Flame F. While the actual velocity profiles are parabolic in shape, for the sake of comparison they are listed in terms of bulk velocity below.

- Coflow velocity – 0.9 m/s
- Flame D
  - Jet velocity – 49.6 m/s
  - Pilot velocity – 11.4 m/s
- Flame F
  - Jet velocity – 99.2 m/s
  - Pilot velocity – 22.8 m/s

**Figure 5.1** is a close-up view of the physical burner extracted from the Sandia Flame reference document (Barlow & Frank, 2007). This image is taken from the base of the flame in order to show the pilot in reference to the fuel jet.
The fuel, pilot and coflow streams are equivalent between the different flame configurations. By increasing only the velocities, the effects of turbulence can be evaluated without additional factors being added. The coflow is air at 274K, the fuel is a mixture of 75% air and 25% CH₄ by volume at 274K, and the pilot composition is comprised of the mass fractions illustrated in Table 5.1. Even though the actual pilot has other species in trace amounts, for modeling purposes, these values are sufficient for combustion to occur in a reduced chemical mechanism.

Figure 5.1 Close-up of Sandia piloted flame burner (Barlow & Frank, 2007)
Table 5.1 Initial Mass Fractions for pilot composition in piloted Methane Jet flame

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Y_{N_2})</td>
<td>0.7342</td>
</tr>
<tr>
<td>(Y_{O_2})</td>
<td>0.0540</td>
</tr>
<tr>
<td>(Y_O)</td>
<td>7.47 \times 10^{-4}</td>
</tr>
<tr>
<td>(Y_{H_2})</td>
<td>1.29 \times 10^{-4}</td>
</tr>
<tr>
<td>(Y_H)</td>
<td>2.48 \times 10^{-5}</td>
</tr>
<tr>
<td>(Y_{H_2O})</td>
<td>0.0942</td>
</tr>
<tr>
<td>(Y_{CO})</td>
<td>4.07 \times 10^{-3}</td>
</tr>
<tr>
<td>(Y_{CO_2})</td>
<td>0.1098</td>
</tr>
<tr>
<td>(Y_{O_2})</td>
<td>0.0540</td>
</tr>
<tr>
<td>(Y_{CO_2})</td>
<td>0.1098</td>
</tr>
<tr>
<td>(Y_{OH})</td>
<td>2.8 \times 10^{-3}</td>
</tr>
<tr>
<td>(Y_{NO})</td>
<td>4.8 \times 10^{-6}</td>
</tr>
</tbody>
</table>

Mixture fraction is the conservative scalar of choice to model non-premixed combustion, so it is important to consider the values associated with the different regions of the flow. By definition, the mixture fraction for the fuel stream is unity and the mixture fraction for the co-flow is zero. Following the logic outlined in Section 2.2, with the mass fractions listed in Table 5.1, the mixture fraction of the pilot stream is \(Z_{pilot}=0.275\). The stoichiometric mixture fraction can be found by considering the stoichiometric fuel reaction with air.

\[
\text{CH}_4 + 2(O_2 + 3.762\text{N}_2) \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 7.542\text{N}_2
\]  

(5.1)

The mass fractions associated with the stoichiometric mixture in Eq. (5.1) are \(Y_{\text{CH}_4}=0.055\), \(Y_{O_2}=0.22\), and \(Y_{N_2}=0.725\). Applying the logic from Section 2.2, again, with these values the stoichiometric mixture fraction is \(Z_{st}=0.365\). While this value isn’t a necessary input for the ODT or LES models, it is useful when analyzing the results.

5.4 Available Experimental Data

The available data from experiments that match the selected model domain must be considered when choosing the terms and structure collected from model simulations. Of most
importance when analyzing a non-premix combustion simulation are the temperature and mixture fraction. These values provide a good view of the overall flame structure, making them excellent comparisons for basic model validation. Additional scalars, such as mass fractions of intermediate species and saturated combustion products, are useful for more in-depth analysis, including reaction completeness and flame structure complexity. The TNF Sandia flame data is a complete set of scalars, which includes mixture fraction, temperature and selected mass fractions measured in experiments. These scalars and their fluctuations are organized and saved as axial profiles, radial profiles and scatter plots, providing multiple views which validate detailed aspects of the flame. The radial profiles and scatter plots are listed at preselected axial distances $x/d$ equal to 7.5, 15, 30, 45 and 60 because the near field and downstream characteristics vary for each of the flame types. The axial profiles range from $x/d = 1.0$ up to $x/d = 75$. It is important to note that the axial and radial profiles are time averages datasets much like the RANS averaging process. Having the data aggregated as such removes many of the fluctuations, causing the curves to appear smoother and slightly dampened. When accumulating data from ODT and LES simulations, the results must also be time averaged in order to create equivalent datasets.

### 5.5 Stand-alone ODT for non-premixed Sandia Flame

ODT simulations of the Sandia Flames D and F represent an axisymmetric cross section of the piloted jet where the segments of the 1D domain are the fuel, pilot and coflow. Three sets of inputs are required to model the Sandia Flame via ODT:

- The inlet conditions defining the fuel stream, the pilot and the co-flow composition
- Reduced reaction mechanism for a CH$_4$-air reaction
ODT model parameters needed to simulate the corresponding turbulence conditions

The inlet conditions for velocity, temperature and species mass fraction are set in accordance with the Sandia Flame conditions outlined in Section 5.3. The scalar quantities are set directly, while the velocity is set using a cubic spline interpolation to accomplish a parabolic velocity curve, which is typical of a round jet.

The mixture of 25% CH$_4$ and 75% air by volume results in mass fractions for CH$_4$, N$_2$ and O$_2$ of Y$_{CH_4} = 0.1563$, Y$_{N_2} = 0.6472$ and Y$_{O_2} = 0.1965$ respectively. Likewise, the air in the co-flow is a typical N$_2$-O$_2$ mixture having mass fractions of Y$_{N_2} = 0.7580$ and Y$_{O_2} = 0.2420$. The CH$_4$-air reaction is modeled with the 15 step GRI 3.0 mechanism defined by (Sung, Law, & Chen, 2001). This mechanism includes 4 elements, 19 species and the reactions outlined in Table 5.2.
Table 5.2 GRI 3.0 Reduced CH₄ Chemical Mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>2H + 2OH = 2H₂ + O₂</td>
<td>CH₂O = H₂ + CO</td>
</tr>
<tr>
<td>2H = H₂</td>
<td>O₂ + C₂H₂ = H₂ + 2CO</td>
</tr>
<tr>
<td>H + HO₂ = H₂ + O₂</td>
<td>OH + C₂H₄ = H₂ + CH₃ + CO</td>
</tr>
<tr>
<td>H + H₂O₂ = H₂ + HO₂</td>
<td>C₂H₆ = H₂ + C₂H₄</td>
</tr>
<tr>
<td>OH + CH₃ = H₂ + CH₂O</td>
<td>H + OH = H₂O</td>
</tr>
<tr>
<td>H + CH₄ = H₂ + CH₃</td>
<td>2NO = O₂ + N₂</td>
</tr>
<tr>
<td>H + OH + CO = H₂ + CO₂</td>
<td>H₂ + CO + NO = H + O₂ + HCN</td>
</tr>
<tr>
<td></td>
<td>3H + H₂O + NH₃ = 4H₂ + NO</td>
</tr>
</tbody>
</table>

The 15-step mechanism is a 12-step CH₄ mechanism augmented with the NH₃ and NO reactions to provide a very limited ability to model NOₓ formation. While NOₓ formation is not the focus of this research, it is included for completeness.

The ODT model parameters corresponding to the Sandia piloted jet flame are expected to generate the statistical equivalent of turbulent conditions. As stated in Chapter 2, the free parameter A corresponds to the amount of energy necessary to generate an eddy at a randomly selected location, and β determines the extent to which the eddies expand the turbulent flow field. For the modeled Sandia flames, A is set to 0.334 and β is set to 1.45. These values combined with the parameters controlling the likelihood of an eddy event are sufficient to cover all of the ranges of turbulence seen within the Sandia Flame family. The jet velocity and the jet Reynolds numbers are the additional input parameters which specify the available turbulent energy within the system. For the Sandia Flame D, the Reynolds number is 22500 and the bulk jet velocity is 55.5 m/s, and for the Sandia Flame F, the Reynolds number is 44500 with a bulk jet velocity of 99.95 m/s. These values provide the velocity gradients and the
turbulent energy needed to activate the selection logic within the stochastic portion of the ODT solution.

The velocity profile is a pseudo parabolic curve, which is the result of a 1D spline constructed through a sample set of points specifying the velocity magnitude located a given radial distance. The radial distance is a relative value, starting at the inner radius of a particular region within the inlet conditions. For the fuel the starting location is the origin. For the pilot the starting location is the radius of the inner portion of the pilot. Table 5.3 lists the scalar velocity factors at given positions, and the inlet velocity is an arbitrary maximum multiplied by this factor. The third column is a number indicating the turbulent character in that part of the region. It is assumed to be proportional to \( u'u' \).

**Table 5.3** Velocity spline definition with turbulent intensities for Flame D and F

<table>
<thead>
<tr>
<th>Radius factor</th>
<th>Velocity factor</th>
<th>Fluctuations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>1.000</td>
<td>0.0309</td>
</tr>
<tr>
<td>0.065</td>
<td>0.999</td>
<td>0.0307</td>
</tr>
<tr>
<td>0.130</td>
<td>0.995</td>
<td>0.0327</td>
</tr>
<tr>
<td>0.194</td>
<td>0.988</td>
<td>0.0366</td>
</tr>
<tr>
<td>0.259</td>
<td>0.978</td>
<td>0.0409</td>
</tr>
<tr>
<td>0.324</td>
<td>0.967</td>
<td>0.0450</td>
</tr>
<tr>
<td>0.389</td>
<td>0.951</td>
<td>0.0504</td>
</tr>
<tr>
<td>0.453</td>
<td>0.933</td>
<td>0.0550</td>
</tr>
<tr>
<td>0.518</td>
<td>0.912</td>
<td>0.0604</td>
</tr>
<tr>
<td>0.583</td>
<td>0.887</td>
<td>0.0648</td>
</tr>
<tr>
<td>0.648</td>
<td>0.858</td>
<td>0.0693</td>
</tr>
<tr>
<td>0.712</td>
<td>0.824</td>
<td>0.0726</td>
</tr>
<tr>
<td>0.777</td>
<td>0.785</td>
<td>0.0773</td>
</tr>
</tbody>
</table>
Each of the numbers defined for the velocity spline are normalized, and thus the same table can be applied to Flame D as well as Flame F velocities. For Flame D, the maximum velocity is set to 62.5 m/s, and for Flame F, the maximum is set to 116.5 m/s, which corresponds to bulk velocities of 49.5 and 99.2 respectively. The pilot and co-flow velocities follow a similar pattern, where the bulk velocities are 11.4 m/s for the pilot of Flame D, and 22.8 m/s for the pilot of Flame F. The co-flow velocity is 0.9 m/s for both flame types.

### 5.6 ODT Statistics

It has been determined that around 200 realizations of ODT simulations, advanced to a time corresponding to an equivalent downstream distance greater than $x/d=100$, providing a sufficient amount of data for the statistics needed from the key flame regions. With a sampling of the data generated from these ODT simulations, the contained statistics are shown to demonstrate the viability of using these simulations for input into LES closure. Figure 5.2 shows the density contour plot rendered from the samples generated from a number of Flame F simulations. The white regions are portions of the state-space where there are no samples. Three key portions of the state-space are without any samples: the upper left, upper right and lower center sections. As these areas are typically far away from the flame, they can be handled

**Table 5.3 Continued**

<table>
<thead>
<tr>
<th>Radius factor</th>
<th>Velocity factor</th>
<th>Fluctuations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.842</td>
<td>0.732</td>
<td>0.0863</td>
</tr>
<tr>
<td>0.907</td>
<td>0.613</td>
<td>0.1230</td>
</tr>
<tr>
<td>0.972</td>
<td>0.291</td>
<td>0.0991</td>
</tr>
<tr>
<td>1.000</td>
<td>0.000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>
with the procedures described in Chapter 4 for interpolating and completing the sample datasets. As is expected with a non-premixed flame, the density shows a strong dependence on temperature with only a slight dependence on mixture fraction. This pattern is mainly due to the minor difference in molecular weights between the fuel stream and the oxidizer stream.

![Density Contour plot](image)

**Figure 5.2** Density Contour plot conditioned on mixture fraction and temperature from un-processed ODT statistics for Flame F simulation

Representing data within the state-space is simply a matter of plotting selected values from the already generated state-space vectors; however, producing spatial plots for ODT simulations requires determining the downstream location, which is an approximate calculation at best. As previously stated in Section 3.6, the downstream distance is a function of the expired time and the bulk velocity. What makes this process an approximation, is that the bulk velocity varies for each time iteration as well as the time difference. In addition, only
select time iterations are saved for visual post processing. Thus, the downstream location is estimated based on an accumulation of velocities multiplied by the time differences from each of the spatial 1-D domains. Figure 5.3 is a characteristic view of the flame centerline cross section for Flame F. It is rendered by assembling several iterative sequences at selective time steps. These views are only intended to illustrate the statistical nature of the data because they are not very effective at portraying the actual flame. From these plots, several characteristics are notable. The flame is more tightly held together in the near field, but it widens, becoming more random downstream. The spreading expected for a turbulent jet is evident in the wider more chaotic field downstream view. In addition, there is a small number of instances of extinction in the outer regions of the near field plot on the left, with the downstream view on the right exhibiting a much higher degree of extinction. Finally, the asymmetric nature of the downstream view as compared to that in the near field shows the statistical variability expands as the simulation progresses. As these properties are expected in the LES simulation, having these characteristics present in the sample data is necessary to verify that the model data will work as expected. Further evidence can be seen in axial and radial plots using the same data samples.
Figure 5.3 Rendered cross section view of ODT simulation for Flame F at in selective approximate downstream regions.
The next analysis to validate the viability of the ODT simulations are axial and radial profiles of temperature and mixture fraction. This type of analysis is similar to the spatial views as above, but they are collapsed into a single view in the specified direction. The axial view is a single curve along the centerline, and the radial profiles are curves expanding radially at different downstream distances. Once again the downstream location is an approximation, and in some cases the available samples are at slightly different locations than what is represented in the experimental data. Figure 5.4 shows the axial profiles for mixture fraction and temperature, and Figure 5.5 and Figure 5.6 show the radial profiles for the mixture fraction and temperature, respectively. In Figure 5.4, the mixture fraction follows the experimental data as well as expected considering the conditions of the data collected. The same can be said for the temperature, however, the maximum is slightly off from experiments downstream from the flame tip. This pattern could, possibly, be explained by looking again at Figure 5.3 to see that the downstream view appears to have the flame data slightly shifted to the right. With a small sample size and data only collected from the centerline, much of this shifted information would not be included in Figure 5.4.

Figure 5.5 shows the mixture fraction profiles at \( x/d = 15, 30, 45 \) and 60. Theses plots are most accurate in the \( x/d = 30 \) and \( x/d = 45 \) locations, mainly because these locations align better with available ODT data; however, the other regions are still in the ballpark of what is expected. With a few anomalies, these plots are in good agreement with experimental data, showing the ODT simulations transport the conserved scalars well enough to capture characteristic behavior. Figure 5.6 shows corresponding plots for temperature at the \( x/d = 15, 130, 45 \) and 60. With the exception of the centerline temperature at \( x/d = 45 \), these also show
good agreement with experiments. Having these plots demonstrate similar patterns to those seen in experiments also shows that the ODT simulation is transporting the reactive scalars well, and can capture any necessary statistics that are contained.

**Figure 5.4** Axial profile of mixture fraction and temperature for ODT simulation of Flame F
Figure 5.5 Radial profiles of mixture fraction from ODT compared with from Barlow and Frank experiments at downstream distances of $x/d=15,30,45$ and 60
Finally, the conditional statistics viewed in state-space show the qualitative nature of the state vectors, and how well they can capture the necessary content for LES closure. In visually analyzing doubly conditioned scalars, both the patterns and the magnitudes of the scalars are considered. **Figure 5.7 through Figure 5.14** show doubly conditioned species mass fractions from ODT compared with those taken from experiments. Both sets of data are constructed by re-organizing spatial profiles in terms of mixture fraction and temperature. In
the fuel and oxidizer plots (Figure 5.7 and Figure 5.8), there is moderate agreement between the experimental and predicted values; however, looking closely at the area around where the flame is expected to reside (1500K < T < 2100K and 0.2 < Z < 0.4) there are subtle differences in the iso-lines illustrating the functional dependence of the mass fractions and the conditioning scalars. As seen in the remaining plots, these patterns are consistent throughout all the conditioned species contours, meaning they are a distinct characteristic of the reaction mechanism and its application to ODT. Albeit slight, the differences in iso-lines produce sensitivity and slight discrepancies in predicted species values.

Looking at the predicted species mass fractions for combustion radials (CO, OH and H₂) seen in Figure 5.11 through Figure 5.13, there are differences between predicted and experimental values that go beyond the iso-lines defining the functional dependence. The predicted values for CO and H₂ follow very similar patterns, where they appear to be overstated in the location x/d=15 and under stated in the location x/d=45. With the values appearing very close in the location x/d=30, one could conjecture that the reaction mechanism within ODT predicts these radials best in the active portions of the flame leading up to the flame tip. The conditioned contours for OH have a pattern that is much different than any of the other species. As expected, OH appears to be concentrated below the adiabatic flame temperature, close to the stoichiometric mixture fraction. This means that the radical shows up as the reaction progresses from ignition through to completion. The predicted values, here, appear to have a larger footprint, as well as higher values, close to the flame tip (x/d=45). These properties seem to indicate that the model is not consuming the radicals at the rate expected. Surprisingly, the predicted contours for NO species mass fraction are reasonably close to experimental values, as seen in Figure 5.14. Granted, the values are over predicted in both x/d=15 and
$x/d=30$, but the values are closer in $x/d=45$ and the patterns match well throughout. The Chen mechanism for methane combustion is known for significant departures in NO prediction, thus the NO variations are not surprising (Barlow, Karpetis, Frank, & Chen, 2001). However, in light of this shortcoming, the results are reasonably good. As these results are indicative of the contents of the closure model for dependent scalar predictions, one would not expect the prediction capabilities to go too far beyond what is viewable in this analysis. However, as predicted values in the filtered LES domain have many different inputs, these predictions should only be considered as background detail when explaining LES results.
Figure 5.7 Comparison between ODT and experiments of conditional statistics for CH$_4$ species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$. 
Figure 5.8 Comparison between ODT and experiments of conditional statistics for O$_2$ species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$
Figure 5.9 Comparison between ODT and experiments of conditional statistics for H$_2$O species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$
Figure 5.10 Comparison between ODT and experiments of conditional statistics for CO$_2$ species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$
Figure 5.11 Comparison between ODT and experiments of conditional statistics for CO species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$.
Figure 5.12 Comparison between ODT and experiments of conditional statistics for OH species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$
Figure 5.13 Comparison between ODT and experiments of conditional statistics for H$_2$ species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$
Figure 5.14 Comparison between ODT and experiments of conditional statistics for NO species mass fraction at downstream distances of $x/d=15$, $x/d=30$ and $x/d=45$
5.7 Kernel Density functions for ODT Distributions

A precursor to building the kernel density functions for LES closure, is the collection and representation of non-parametric distributions that are characteristic of the ODT simulations. As described in Section 4.5, the histogram distributions that represent ODT data are in the form of normalized counts of data samples at locations in the state-space. These collection counts can be illustrated using a bar graph, which shows the value at each location as a bar on the plot. After performing the kernel fitting routine, the resulting distribution is in the form of a non-linear regression, which is best represented with a line graph. Figure 5.15 through Figure 5.18 demonstrate the transformation from the discrete histogram distribution to the continuous KDF for selected means, using data from Flame D and Flame F simulations. $\tilde{\theta}_T$ is the normalized temperature, making the distribution scales match for temperature and mixture fraction. There are several things to note about these graphs. First, in all cases the KDFs shown are good representations of the given histogram, without exhibiting drastic discontinuities. The plot of $P(\tilde{Z} = 0.5)$ at $Log_{10}(\tilde{Z}/\tilde{Z}^\alpha) = -1.0$ in Figure 5.15 shows a good example of how the KDF captures the essence of the underlying data, without giving certain points too much weight. In all cases, the distributions appear more Gaussian for the smaller variances, and show more dynamic behavior for the higher variances. Additionally, there appears to be a trend showing that higher variances temperature distributions are more skewed while the mixture fraction distributions are more multi-modal.
Figure 5.15 Histogram and KDF distributions from ODT data at $\bar{Z}=0.1$ and $\bar{Z}=0.5$ for Flame D simulation. Note that the scale is different in the bottom two rows.
Figure 5.16 Histogram and KDF distributions from ODT data at $\tilde{Z}=0.1$ and $\tilde{Z}=0.5$ for Flame F simulation. Note that the scale is different in the bottom two rows.
Figure 5.17 Histogram and KDF distributions from ODT data at $\tilde{\theta}_T$=0.1 and $\tilde{\theta}_T$=0.5 for Flame D simulation. Note that the scale is different in the bottom two rows.
Figure 5.18 Histogram and KDF distributions from ODT data at $\tilde{\theta}_T=0.1$ and $\tilde{\theta}_T=0.5$ for Flame F simulation. Note that the scale is different in the bottom two rows.
5.8 Distribution Analysis

The distributions shown in the previous section are compared with an equivalent $\beta$-PDF to see how the learned multi-modal KDFs matches up with the prescribed single point distribution. Figure 5.19 through Figure 5.22 show comparisons of the KDF distributions learned from ODT simulations with the $\beta$-PDF having an equivalent set of properties. When the variances are small the ODT distributions tend to be more symmetric and consistent with the $\beta$-PDF. With the smaller variance distributions, ODT exhibits a smaller standard of deviation, and thus it is questionable whether there is a limitation in the spread of the distribution data, or if the corresponding $\beta$-PDF is including too much data for that portion of the state-space. At the higher variances, the learned distributions are much more skewed in the center regions but seem to still contain the asymmetric shape of the $\beta$-PDF in the outer regions. Once again, the $\beta$-PDF is incapable of representing the true shape of the higher variance distributions. The KDFs learned from ODT realizations on the other hand illustrate bimodal curves that are more representative of the Sandia Flame results.

The $\beta$-PDF has two main limitations when being used to match the distributions of turbulent scalars: the data range limitations may not best fit realistic ranges for actual scalar variances, and the distribution curves may not best fit the patterns seen in turbulent flows. These issues are very evident in the figures comparing the different types of distributions above. For lower values of scalar variances, the $\beta$-PDF isn’t capable of rendering a curve with a matching standard deviation. In the plots constructed from higher variance values, the $\beta$-PDF are better matched in regards to statistical character; however, the actual distributions for these ranges are more skewed and less Gaussian. From these comparisons, the reasons for choosing a more realistic distribution in tabulation based closure models are very evident. The
more the scalar distribution matches the actual distribution for a given scalar vector the better the table can predict values for filtered quantities. In contrast, the β-PDF does provide smooth evenly distributed values which in some cases can be desired. For this reason, the β-PDF is still valid for certain applications.

While the KDFs learned from ODT have shown to contain more turbulence induced features than the β-PDF, a similar comparison with experimental results is necessary to validate the ability to model sub-grid flame PDFs. Looking back at the experimental distributions shown in Section 4.1, the basic trends and large scale functional characteristics appear to be similar to those seen in the shapes illustrated in Figure 5.19 through Figure 5.22. In contrast, however, there are differences in both the format of the data as well as the shapes of the ODT distributions that require attention. First, the experimental distributions in Section 4.1 are the result of data collections gathered at specific locations in the flow field whereas the ODT distributions include samples from the entire domain. For the temperature distributions the, experimental results in Figure 4.1 are conditioned on mixture fraction in the range of $0.3 < Z < 0.4$. In this research, the temperature and mixture fraction are assumed statistically independent, and as a result, the temperature distributions in Figure 5.21 and Figure 5.22 cover the entire range of mixture fraction values. Finally, the experimental distributions in Figure 4.2 through Figure 4.4 illustrate the composition of the mixture using individual species mass fractions, while the ODT distributions illustrate the mixture through the mixture fraction. Consequently, the mixture fraction distribution, which contains the collective information of all of the distributions present in the mixture, includes more information.

When directly comparing the temperature distributions in Figure 4.1 with those in Figure 5.21 and Figure 5.22 there is evidence to support the claim that the ODT distributions
are better models of the experimental distributions than the prescribed β-PDF. Even though there is not enough information to draw direct correlations between the conditionally averaged distributions from Figure 4.1 and those at specific variance levels in Figure 5.21 and Figure 5.22, an attempt to align the illustrations can ensue by looking at the axial and radial profiles of temperature variance in Figure 8.1, Figure 8.3, Figure 8.4, and Figure 8.6 of Sections C1 and C2 in the Appendix. In the axial variance plots it appears that the temperature variance peaks at around $x/d=30$, but the radial plots show that the temperature variance is higher for $x/d=15$ than for $x/d=30$. This information combined with the observation that mixture fraction variance is higher at $x/d=15$ in Figure 7.26 leads to the supposition that plots for $\text{Log}_{10}(\overline{T'_T}) = 5.80$ in Figure 5.21 and Figure 5.22 correspond more with plots for $x/d=15$ in Figure 4.1; however, the primary shapes of the KDFs in Figure 5.21 and Figure 5.22 are more like those for $x/d=30$ in Figure 4.1. This correlation leads to the conclusion that ODT distributions are limited in the variance that can be captured in relation to the experimental results. Shortcomings aside, the KDF plots for temperature at $\text{Log}_{10}(\overline{T'_T}) = 5.80$ have very similar shapes to those from the experimental distributions at $x/d=30$ and show hints of the multi-modal characteristics seen in the $x/d=15$ experimental distributions. The biggest issue in the $\text{Log}_{10}(\overline{T'_T}) = 5.80$ plots of Temperature KDF for Flame F is that the statistical variability is less defined than that seen in Figure 4.1, which is evidence that there is a larger amount of frequency noise in the ODT distributions. While the reasons for this noise require investigation, methods to minimize the impact need to be addressed. Some of the noise can be mitigated slightly by increasing the kernel width used in the KDF; however, there is delicate balance between losing the information found in the peaks with eliminating the noise. A better strategy would be to either determine if the noise can be reduced within the ODT simulation.
or if a post processing step between collection and KDF learning can reduce the noise without too much information loss. It is important to note, however, that a more realistic distribution with a manageable amount of noise is still better than the prescribed distribution when attempting to capture complex flame characteristics.

While there isn’t a direct correlation between the temperature KDFs at lower variance levels, some characteristics of the plots for temperature distribution at $\log_{10}(\overline{T'^2}) = 5.375$ can be discussed. First, as the variance is reduced from the maximum, the spread of temperature distribution is much more defined which is similar to the change seen in Figure 4.1 in the difference from $x/d=15$ to $x/d=30$. The discrepancy to note is that the ODT distributions plots for both Flame D and Flame F show similar dissipation whereas, this pattern is only notable in the Flame F plot of Figure 4.1. This difference suggests that the amount of turbulent energy present in the Flame D ODT simulation is slightly higher than that which is present in the experiments. In addition, while the ODT distribution for Flame F shows hints of dual modality, the second mode is less evident than that seen in the plots in Figure 4.1. This difference implies that the information captured from the ODT simulation is either incomplete or oversaturated. Several factors could play into this issue. First, the filter width used to generate the correlated vectors could either be too large or too small to see this additional information. As the filter width is fixed and there are no comparisons showing the effects of the filter width this conclusion is difficult to ascertain. Future work would be necessary to confirm this possibility. A similar issue exists with the granularity of the variance indices. These preselected values for the number of variance buckets may cause the distributions to overlap what is seen in ODT with what is observable in experiments. Finally, the differences could be the results of the parameters selected for the ODT simulations. Similar issues are
apparent in the ODT plots at the lower variance with regards to noise; however, they don’t appear to be as severe or appear to change the modality of the distribution.

A thorough comparison of the mixture fraction KDFs in Figure 5.19 and Figure 5.20 with the conditional PDFs for species mass fractions in Figure 4.2 through Figure 4.4 requires more information than is available from this study; however, as the mixture fraction represents the chemical state of the mixture, the mixture fraction KDF also represents the statistical nature of the mixture. Figure 4.2 through Figure 4.4 show 3 distinctly different patterns which are observable in some form in the mixture fraction KDFs for both Flame D and Flame F. The H$_2$O distributions in Figure 4.2 look more like the temperature distribution than they do the mixture fraction, but the separation of the two distinct modes can be seen slightly for $Log_{10}(\overline{Z'Z'}) = -1.425$ and more definitely for $Log_{10}(\overline{Z'Z'}) = -1.0$ in Figure 5.20 for Flame F. A similar pattern to the OH distribution in Figure 4.3 can be seen in the $Log_{10}(\overline{Z'Z'}) = -1.0$ plot in Figure 5.19 for Flame D where the distribution is skewed into the lower boundary. This characteristic is slightly odd because is it less evident in the plot for Flame F, but the two simulations do share similar parameters, and thus they exhibit the same statistical character in the ODT domain. The plot that appears to agree best with the mixture fraction KDFs is the CO distribution shown in Figure 4.4. The CO distribution demonstrates the spreading of two distinct modes in the higher variance $x/d=15$ region which is also evident in the mixture fraction KDF for $Log_{10}(\overline{Z'Z'}) = -1.0$ in Figure 5.20 for Flame F. Interestingly, the noise seen within the mixture fraction KDFs at higher variance is also observable in the CO distribution. While the shapes of the KDFs cannot be matched to a specific mass fraction cPDF, commonalities between each of the individual species are evident,
thus providing further support that the mixture fraction KDF is capturing the statistical nature of the chemical state better than a prescribed PDF.

One characteristic that is notable in all the mixture fraction plots at the higher variances is the noise. Even though the experimental distributions contained noise as well, the different modes are more discernable. With the mixture fraction KDF these modes are less distinct and may appear as higher amplitude noise. The plot for $Z=5.0$ at $\log_{10}(Z^2) = -1.0$ in Figure 5.20 for Flame F looks as though there are two modes represented; however, the noise in the lower values of $Z$ may be perceived as additional modes to be included. Further research is required to determine what the additional noise is reporting as well as how to articulate the source of the noise. Given the distributions as they are, care must be taken when applying them to closure tables. There are three methods that can be applied to deal with the noise. First, the KDE can be adjusted with a larger width kernel resulting in a smoother distribution with less chance for falsely reported modality. Unfortunately, picking a filter width that is too large is detrimental because it removes much of the statistical information available. Another approach is to apply a more traditional low-pass filter removing the disturbances which are large enough to be perceived as an additional mode but not the others. Once again, without knowing which information is important, arbitrarily removing frequencies may not be the best approach.

Finally, the granularity and ranges of valid variances indices can be adjusted to determine the best selection for each distribution represented. Covered in more detail in Section 4.5, adjustments with the variance ranges are limited to how much optimization can be accomplished due to the amount of sample data needed to build quality distributions. In the current study, the distribution indices illustrated in Figure 5.19 through Figure 5.22 are used
with the LES closure tables for source terms and density needed in the LES simulations, but minor adjustments are applied to improve the representation of the species mass fractions calculated in post processing. Even though the effectiveness is limited, these adjustments reduce the noise and unwanted modality such that post processing results are improved. Interestingly, such adjustments were found to be less effective when used with the LES source terms and density. This difference in effectiveness is believed to be because the species mass fractions are biased to their own distributions causing the tabular lookup to be more sensitive to errors in the mixture fraction KDF. Further research to quantify this sensitivity may be helpful in determining if a single conservative distribution is sufficient to predict these quantities, or if additional scalars are needed for best results.
Figure 5.19 Comparison of KDF with β-PDF at $\bar{Z}=0.1$ and $\bar{Z}=0.5$ for Flame D simulation. Note that the scale is different in the bottom two rows.
Figure 5.20 Comparison of KDF with $\beta$-PDF at $\tilde{Z}=0.1$ and $\tilde{Z}=0.5$ for Flame F simulation. Note that the scale is different in the bottom two rows.
Figure 5.21 Comparison of KDF with $\beta$-PDF at $\bar{\theta}_T=0.1$ and $\bar{\theta}_T=0.5$ for Flame D simulation. Note that the scale is different in the bottom two rows.
Figure 5.22 Comparison of KDF with β-PDF at $\bar{\theta}_T=0.1$ and $\bar{\theta}_T=0.5$ for Flame F simulation. Note that the scale is different in the bottom two rows.
In summary, studies that predict fluid motion resulting from stochastic processes must
best choose how to represent those processes within the framework of the solution. A priori
decisions based on simple models may be a reasonable choice, but such choices are generally
limited in both implementation and accuracy. With advancements in experimentation and
numerical solutions, collection of data needed to measure statistics is becoming less and less
of an issue. Therefore, the challenges facing modern research are the processes by which
scientists turn this information into useful and accurate distributions. Application and
exploration of these processes enables further advancement of turbulent reacting models by
removing pre-existing limitations with prescribed distributions. Applying Kernel Density
Functions learned from data collected with the procedures described above is a preliminary
step to evaluating what gains are possible when switching from prescribed distributions to
those sourced from highly resolved data. Care must be taken, however, to not carte blanche
apply data to a model. Without confirmation that the representative distributions contain
minimal errors, further application could be misleading.
6 LES Results for Sandia Flame D

6.1 Flame D Introduction

The Sandia Flame D is modeled with LES using a custom OpenFOAM application, which includes the LES closure table described in Section 4.8. Covered in Appendix A, the OpenFOAM application solves the transport equations described in Chapter 3 on a 3D polyhedral mesh, applying the boundary conditions outlined in Sections 5.3 and 5.5. Flame D is turbulent enough to require a complete model, but not so intense that many of the typical model assumptions, such as scale separation and finite chemistry, aren’t of big concern. Even though simulations applied to the Flame D setup aren’t necessarily differentiating, they are necessary as a baseline to determine that the model can perform as well as other available methods. As stated previously, there are three basic ways with which to compare the modeled results from experimental data. The first plots shown are the velocity profiles and several cross-section views. While there aren’t any comparisons with these views, they do provide some detail into the overall character of the flame. Axial profiles of mixture fraction, temperature and other scalars, along with RMS values, are compared with experimental results. To complete the details of the flame further, radial profiles of scalar and RMS values are evaluated in the same domain, then finally the conditioned scalars at selected locations downstream are considered. With each of these result sets, analysis searches for the existence of extinction and re-ignition along with positive and negative properties of the model.
6.2 Mesh definition and Boundary Conditions

As described in Chapter 5, this flame is an axial jet with a concentric pilot flame, surrounded by a cold co-flow of air. The geometry in the LES mesh closely matches those seen in experiments. This mesh is comprised of polyhedral cells with polygon faces, and the inlet velocity for each region of the lower boundary is set based on the experimental setup described in Section 5.5. In order to simulate the necessary turbulent energy, a boundary condition which can introduce velocity fluctuations is required for the jet and the pilot. Several methods are available, but the boundary condition applied, here, is a simple combination of a fixed parabolic velocity and fluctuating term which is proportional to a reference field. The reference field is the unchanged fixed velocity, and the resulting boundary is balanced with an RMS correction, ensuring that the resulting RMS velocity does not exceed what is expected. The remaining boundary conditions are explained in Appendix A5.

6.3 Flame D Velocity Profile

Analyzing the radial velocity profile provides insight into the velocity gradients that drive turbulence through most of the flame regions. Figure 6.1 shows the radial profiles of the streamwise velocity along with the RMS value. The velocities and RMS values are normalized by the centerline velocity so that the scales match between Flame D and Flame F. At $x/d=2$, the flow is still dominated by the inlet boundary condition because the profile is very close to the inlet condition and the RMS values are very low. At $x/d=15$, the velocity gradients are still very steep, but the effects of the boundary are lessened as the RMS increases due to turbulent fluctuations. Finally, the RMS values gradually increase downstream as the radial profile becomes more self-similar. The self-similarity profile seen at $x/d=60$ and beyond is
very characteristic of an axisymmetric diffusion jet, which is the result of the spreading flame entraining cold fluid from the sides.

**Figure 6.1** Radial profile of axial velocity normalized by the centerline velocity $U/U_c$
6.4 Flame D Cross Section

A visual analysis of the LES flame can also be interesting in the evaluation of the LES-ODT closure model. The cross section views seen in Figure 6.2 through Figure 6.4 give a good visual representation of the flame showing both ignition and re-ignition. In Figure 6.2 the temperature profile exhibits a light degree of flame wrinkling, as well as several pockets where the temperature is lower than surrounding areas. These pockets and the wrinkling effects are characteristics of extinction, leading to the conclusion that this flame is demonstrating a light amount of extension. At around $x/d=30$, there is an area where there is a break in the mixture fraction contour, and the flame temperature is decreased. Then later, the flame is the more consistent and hotter at $x/d=45$ and slightly beyond. Figure 6.3 shows the H$_2$ species profile that corresponds to the temperature in Figure 6.2. Interestingly, the H$_2$ tends to stay almost exclusively inside the Stoichiometric mixture fraction, which means that H$_2$ is only truly a factor in fuel rich portions of the mixture. The predicted values are highest between $x/d=37$ and $x/d=41$, which is right before the flame tip. This area is also where the temperature seems to reduce a bit indicating that higher than normal H$_2$ is seen in this section. The contour plot showing CO$_2$ species mass fraction exhibits a completely different behavior. For the most part, CO$_2$ levels are the highest along the stoichiometric mixture fraction and they match with the flame temperature. As expected, this means that higher levels of CO$_2$ are more prevalent where the reaction is allowed to complete, thus resulting in the higher temperatures.
Figure 6.2 Temperature contour plot on 2D centerline cross section for Flame D. The greyscale line shows the stoichiometric mixture fraction.
Figure 6.3 $Y_{H_2}$ species mass fraction contour plot on 2D centerline cross section for Flame D. The greyscale line shows the stoichiometric mixture fraction and the blue line shows the flame boundary.
Figure 6.4 CO$_2$ species mass fraction contour plot on 2D centerline cross section for Flame D. The greyscale line shows the stoichiometric mixture fraction and the blue line shows the flame boundary.
6.5 Flame D Axial Profiles

Basic flow characteristics are validated by comparing scalar profiles of predicted values along the centerline to equivalent experimental values. Axial profiles are drawn as a function of the distance from the inlet, which is normalized by the jet diameter \((x/d)\). The data provided in the TNF datasets are time averaged ensembles. To support equivalent comparisons, the LES data collected for each of the axial plots are also averaged over time. The number of time slices may vary, but the best results are accomplished with at least 50 different sample sets. With both the mean and RMS values shown, each plot shows how well the ODT-LES method predicts the mixing and combustion characteristics of the flame as they relate to the underlying unsteady motions.

Figure 6.5 shows comparisons of predicted and experimental results for the axial profiles of the mixture fraction, temperature and associated RMS values. From this view, we see that both sets of predicted values follow similar trends to the experimental data, but that there are some slight differences plus or minus along the overall path. While these discrepancies are within acceptable error limits, a discussion concerning the differences is still of value. In the region between \(x/d=15\) and \(x/d=45\), the mixture fraction profile shows that the scalar mixing appears to be increased, resulting in slightly under predicted mixture fraction values. At the same time in the same region the temperature is also slightly under predicted in comparison with experimental values. These two discrepancies are complicated to analyze because of the interdependence between the momentum and the transported scalars, but it is clear that the errors for one variable are consistent with errors in the other. What is seen as accelerated mixing with the conserved scalar is seen as premature extinction with the temperature. This situation is reversed downstream where the temperature and
mixture fraction values are slightly over predicted. This apparent slowing of the mixing process is allowing for the combustion to stay resident slightly longer than expected. In both plots, the RMS values stay reasonably close to the experimental values, indicating the model is capturing turbulent fluctuations within the simulation pretty well. Despite the minor discrepancies, the ODT-LES model has predicted the centerline view of the transported scalars reasonably well, showing that the basic mixing and combustion are being captured.

Figure 6.6 and Figure 6.7 demonstrate the closure model’s effectiveness in predicting scalar terms that are dependent on the transported state vector. The scalars shown in Figure 6.6 and Figure 6.7 demonstrate the same basic trends as those seen in the experimental data. Overall, the profiles line up well with experimental values, but there are a few locations where each exhibits a deviation from what is expected. In Figure 6.6 the fuel matches with experiments pretty well, while the oxidizer is slightly over predicted in the region between $x/d=20$ and $x/d=40$. In light of the analysis of the transported scalars, this would seem to indicate that the prediction of $O_2$ is more sensitive to errors in either the mixture fraction of the temperature. The remaining scalars all follow a similar trend. They are all reasonably accurate from the origin up to the location at $x/d=40$, but then they diverge slightly downstream from there. In this region, $H_2O$ is over predicted while $CO_2$ is under predicted. Both NO and OH are under predicted around the flame tip, and $H_2$ and $CO$ follow almost identical error patterns. They are both over predicted in the region past the flame tip. Some of these discrepancies mentioned above are consistent with errors seen in the transport variables, but others are more likely to be limitations of the reaction mechanism used in the stand-alone ODT. Thus, the errors could be seen as the result of the closure model’s sensitivity to input errors, or errors contained internally in the closure model itself. Similar
to the transported scalars the RMS values are predicted with a decent amount of accuracy, showing this portion of the closure model is good at capturing fluctuations in the dependent scalars. While the ODT-LES models has appeared to perform well in predicting axial profiles, radial plots are analyzed for further evaluation. The next section shows these profiles and discusses the data contained.

Figure 6.5 Axial Profiles of mixture fraction and temperature for Flame D
Figure 6.6 Axial Profiles of CH$_4$, O$_2$, H$_2$O and CO$_2$ Species Mass Fraction for Flame D
Figure 6.7 Axial Profiles of CO, OH, H\textsubscript{2} and NO Species Mass Fraction for Flame D
6.6 Flame D Radial Profiles

To support the analysis of Section 6.5, the radial profiles for scalars seen in Flame D are also analyzed. Figure 6.8 through Figure 6.17 show the radial profiles for the transported scalars as well as the secondary scalars. At first glance, the transported scalars appear to line reasonably well with experimental data, as do the dependent scalars. There are some minor differences in each of the plots that should be discussed. The mixture fraction profile seen in Figure 6.8 matches very closely with experimental values in the nearfield region ($x/d=2$ and $x/d=15$), but separates slightly further downstream ($x/d=30$ and $x/d=45$). The discrepancies between the predicted and experimental mixture fractions in these latter regions are similar to the differences discussed previously around the centerline, where they were shown to be under predicted in one section, but over stated in the next. Temperature, on the other hand, as seen in Figure 6.9, is under predicted at the center part of the flame at the very beginning ($x/d=2$), and then over predicted further downstream ($x/d=15$). The predicted values are more accurate around the flame tip ($x/d=30$ and $x/d=45$), but they also show a slight over/under prediction pattern. This behavior would seem to indicate that the predicted reaction progresses ahead of what is expected early in the flame, but that it returns to normal later, close to the flame tip. One could suggest that this pattern points to a slight delay from what is expected in the prediction of extinction within the turbulent flame, but with the other factors involved this analysis is complex.

The species mass fraction profiles line up well with what is seen in the transported scalar profiles. The fuel species mass fraction (CH$_4$) in Figure 6.10 is accurate up through the flame tip, but with the exception of the flame tip ($x/d=45$), the oxidizer (O$_2$) in Figure 6.11 is mostly over predicted in the radial areas from the flame region and beyond. Predicted
values of the saturated combustion products (CO₂ and H₂O) seen in Figure 6.12 and Figure 6.13 show similar patterns where they are under predicted at the beginning stage (x/d=2), very accurate up through the flame tip at x/d=45, and then diverge past the flame tip. The combustion radicals (CO, OH and H₂) seen in Figure 6.14 through Figure 6.16 are most accurate in the mid-section of the flow (x/d=15 and x/d=30), which is also the most active part of the flame. CO and H₂ are over predicted in the near field (x/d=2), at the flame tip (x/d=45) and beyond while OH is under predicted for these same locations. Consistent with the discussion in Section 5.6, these statements are just as indicative of the reaction mechanism used as they are of the characteristics of model. Finally, predicted NO species mass fraction values in Figure 6.17 are closest to experimental values at x/d=30, but they are over predicted closer to the jet, and under predicted at the flame tip (x/d=45) and beyond. Much of this analysis can be reinforced by examining the species mass fractions in state-space. The next section covers these in more detail.
Figure 6.8 Radial profiles of mixture fraction at $r/d = 2, 15, 30, 45, 60$ ad 75 for Flame D
Figure 6.9  Radial profiles of Temperature at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
Figure 6.10  Radial profile of CH$_4$ species mass fraction at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
Figure 6.11 Radial profile of O$_2$ species mass fraction at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
Figure 6.12 Radial profile of CO\textsubscript{2} species mass fraction at \( r/d = 2, 15, 30, 45, 60 \) and 75 for Flame D
Figure 6.13 Radial profiles of H$_2$O mass fractions at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
Figure 6.14 Radial profiles CO mass fraction at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
Figure 6.15 Radial profile of OH species mass fraction at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
Figure 6.16  Radial profiles of H$_2$ at $r/d = 2, 15, 30, 45, 60,$ and $75$ for Flame D
Figure 6.17 Radial profile of NO species mass fraction at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D
6.7 Flame D – State-Space Analysis

Basic flame characteristics such as scalar transport and global reactions can be evaluated using axial and radial profiles, but determining the statistical nature of the flame requires analyzing variables from the perspective of the key transported variables. This process can be done by plotting the variables in state-space, showing them as a function of mixture fraction. These views collapse the information contained in all the instances of the state variables to show correlations between predicted scalars and the chemical state of the system. Figure 6.18 through Figure 6.25 show the conditioned species mass fractions as a function of the mixture fraction state-space. The conditioning variable for the experimental plots is the instantaneous mixture fraction, while the conditioning variable for the LES plots is the filtered mixture fraction. In both cases, the plots represent ensembles of data collected over different time slices. The calculated profiles line up reasonably well with the experimental results, with a few differences to note. In Figure 6.18 and Figure 6.19, predicted fuel and oxidizer (CH₄ and O₂) values are generally accurate for most of the state-space. Exceptions include the predicted fuel at higher mixture fractions in the near field (x/d=15), and the predicted oxidizer close to the stoichiometric mixture fraction at x/d=15 and x/d=30. The saturated combustion products (H₂O and CO₂) seen in Figure 6.20 and Figure 6.21 also line up well with experimental data showing some minor discrepancies in the regions around the stoichiometric mixture fraction. The combustion radicals (CO and OH) shown in Figure 6.22 and Figure 6.23 are elevated in the flame region in the location at x/d=15, but are more accurate in the other locations. The CO mass fraction exhibits unrealistic behavior in the fuel rich side of the state-space in the regions around x/d=45 and x/d=60. As this range of mixture fraction values is way outside the norm for those axial locations, these results are likely the result of
statistical outliers; thus, these types of errors may be less of a factor in the overall evaluation of the model. Finally, the H₂ and NO mass fractions in Figure 6.24 and Figure 6.25 are also elevated in the flame regions for \( x/d = 15 \), but the plots match up well in the other locations.

These conditional species profiles are excellent examples of what can be predicted using the LES-ODT model, but the results for OH and H₂ in the location at \( x/d = 15 \) warrants a little discussion. This region is where the LES-ODT model appears to struggles the most in predicting the species mass fractions. The elevated values would seem to indicate that the solution is struggling to keep the flame extinct where extinction is expected, but the spatial profiles for that same location would indicate otherwise. This discrepancy would points to shortcomings with the LES-ODT closure in evaluating these secondary scalars, but the source of the issue is unclear. One possible answer is that the conditional species mass fractions are more susceptible to errors seen in the transported state variables. This area between \( x/d = 15 \) and \( x/d = 30 \) is where both the mixture fraction and the temperature drift from experimental results. Due to the under predicted temperature one could certainly conjecture that extinction is present in this region, but the under prediction of mixture fraction is more indicative of a combustion process proceeding too early. Due to the sensitivity of the model to variations in mixture fraction and temperature, slight errors in mixture fraction may produce slightly larger errors in predicted mass fractions. Finally, in light of the discussions in Section 4.1 and Section 5.8, the KDFs included in the LES-ODT closure table may be less effective at predicting these scalars for the highest levels of temperature and mixture fraction variance. The mixture fraction distributions with the higher variances for Flame D in Figure 5.19 show more modes and noise than that seen in the Flame D distribution for OH in Figure 4.3. These differences at the higher variances combined with the results in Figure 6.23 are further evidence that
additional work is necessary to improve the handling of the KDFs learned from ODT simulations. These issues aside, most of the results are within reasonable error levels and give reason to pursue further development.
Figure 6.18  Comparisons of conditional mean CH$_4$ species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame D. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
Figure 6.19 Comparisons of conditional mean O₂ species mass fraction in state-space at x/d=7.5, 15, 30, 45, 60 and 75 for Flame D. Note that “LES-ODT” is conditioned on Z̃, and “Barlow & Frank” is conditioned on Z.
Figure 6.20 Comparisons of conditional mean H$_2$O species mass fraction in state-space at $x/d$ = 7.5, 15, 30, 45, 60 and 75 for Flame D. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
Figure 6.21 Comparisons of conditional mean CO$_2$ species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame D. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
Figure 6.22  Comparisons of conditional mean CO species mass fraction in state-space at $x/d=7.5, 15, 30, 45, 60$ and $75$ for Flame D. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
Figure 6.23 Comparisons of conditional mean NO species mass fraction in state-space at $x/d=7.5, 15, 30, 45, 60$ and $75$ for Flame D. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
Figure 6.24 Comparisons of conditional mean $H_2$ species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame D. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
Figure 6.25  Comparisons of conditional mean NO species mass fraction in state-space at $x/d=7.5, 15, 30, 45, 60$ and 75 for Flame D. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow & Frank” is conditioned on $Z$. 
7 LES Results for Sandia Flame F

7.1 Flame F Introduction

The main difference between the Flame D and Flame F configuration is the inlet velocities. Increasing the inlet velocities of the jet and pilot streams also increases the initial gradients, which in turn increases the statistical uncertainty. In order to model this increased uncertainty numerically, fluctuations are added into the velocity. For ODT simulations, these fluctuations are induced with the probabilities linked to the velocity gradients. Within the LES inlet boundary, the fluctuations are added by superimposing random fluctuations on top of the velocity profile described in Section 5.5. Using the boundary implementation described in Appendix A5, the induced fluctuations are increased for the Flame F simulation in order to better match the expected turbulent velocities. Similar to the analysis of Flame D, Flame F is analyzed through visual plots of velocities and scalars in the spatial domain and scalars in the filtered state-space.

7.2 Flame F Velocity profile

The velocity profile for Flame F is similar in structure to that seen in Flame D, but it is different in subtle ways that are important to the study of turbulent jets. Figure 7.1 shows the radial profile of the streamwise velocity at different downstream locations. Two main differences can be noted. First, the nearfield plot at $x/d=2$ shows that the Flame F velocity is mixing much sooner than the Flame D velocity. Where the Flame D plot shows a structure still resembling the inlet boundary, the Flame F profile is smoother, showing signs of earlier mixing. Likewise, the Flame F profiles are nearing the self-similarity stage much sooner.
than the Flame D profiles. These increased levels of velocity mixing also have an effect on the scalar mixing, which is why Flame F is expected to show more signs of turbulence.

**Radial Profile – $U/U_c$ – Flame F**

**Figure 7.1** Radial profile of axial velocity normalized by the centerline velocity $U/U_c$
7.3 Flame F Cross Section

Spatial contour plots of transported scalars for Flame F reveal a much more chaotic flow than that seen with the Flame D analysis. Figure 7.2 shows the temperature contour as seen in a 2D cross section across the flame, and Figure 7.3 and Figure 7.4 show the H$_2$ and CO$_2$ mass fractions for the same sample set. The first characteristic to note is that the single contour representing the stoichiometric mixture fraction is much more wrinkled in the Flame F sample as opposed to that in the Flame D sample. In the section between $x/d=15$ and $x/d=45$, there are several examples of reductions in the levels of the temperature and mass fractions. These instances appear to be more prevalent where $Z_{st}$ exhibits sharp changes in direction, creating the appearance of pockets or craters. As noted with Flame D, H$_2$ appears to be most dominant on the fuel rich side of $Z_{st}$, but contrary to the example from Flame D, Figure 7.3 shows many more instances of H$_2$ hotspots, implying that there are several key reaction zones, while Flame D shows only a single dominant reaction zone. Similar statements can be made concerning CO$_2$. As with Flame D, CO$_2$ follows closely along with $Z_{st}$, but Figure 7.4 demonstrates that areas where $Z_{st}$ is most distorted are locations where CO$_2$ levels fall off. From these views, it is very evident that the Flame F simulation contains more turbulence and demonstrates higher amounts of extinction. Analysis of other spatial profiles and conditional plots can support this observation.
**Figure 7.2** Temperature contour plot on 2D centerline cross section for Flame F. The greyscale line shows the stoichiometric mixture fraction.
Figure 7.3  H$_2$ species mass fraction contour plot on 2D centerline cross section for Flame F. The greyscale line shows the stoichiometric mixture fraction and the blue line is the outline of the flame.
Similar to the Flame D validation, the axial and radial profiles are analyzed as comparisons with experiment data. Figure 7.5 through Figure 7.7 show the axial profiles for each of the scalars considered with Flame F. Figure 7.5 shows axial profiles for the mixture.

**Figure 7.4** CO$_2$ species mass fraction contour plot on 2D centerline cross section for Flame F. The greyscale line shows the stoichiometric mixture fraction and the blue line is the outline of the flame.

7.4 Flame F Axial Profiles

Similar to the Flame D validation, the axial and radial profiles are analyzed as comparisons with experiment data. **Figure 7.5** through **Figure 7.7** show the axial profiles for each of the scalars considered with Flame F. **Figure 7.5** shows axial profiles for the mixture...
fraction and temperature. As with the Flame D comparison, these scalar and RMS profiles match well with the experimental data, illustrating that the model is capturing the essence of this the non-premixed turbulent combustion well. Both plots in Figure 7.5 exhibit similar types of errors as with Flame D, but in this case they appear to be less pronounced. Other factors aside, seeing an improvement from Flame D to Flame F could highlight the ODT-LES model’s dependence on ODT originated distributions.

Also, similar to the Flame D axial profiles, the profiles of dependent scalars as seen in Figure 7.6 and Figure 7.7 match generally well with experiments with a few minor issues to note. While the Flame D simulation predicted fuel levels better than oxidizer levels, the Flame F simulation demonstrates the opposite. In Figure 7.6, CH$_4$ levels seem to be slightly under predicted for most of the domain, while the O$_2$ levels are much more accurate. Albeit minor, O$_2$ is under predicted just before the flame tip, and over predicted towards the far field boundary; but contrary to the Flame D plots, the overall curve is reasonably accurate. As mentioned before, the sensitivity of the secondary scalar closure tables to input errors plays a large role in prediction of dependent scalar quantities. In this case, the transported scalars appear to be more accurate with Flame F, thus dependent scalars are predicted better. The saturated combustion products (CO$_2$ and H$_2$O) are both over predicted slightly in the middle portions of the flow, but their shapes are more consistent and better match experiments than do those in the Flame D example. As seen in Figure 7.7, the same can be said for the radials CO, OH and H$_2$. All three curves line up well with experiments with the exception of the center part of the OH curve. Close to the flame tip, OH levels are under predicted towards the jet, and they are slightly distorted. Also in Figure 7.7, NO levels leading up to the flame tip
are predicted well, but they fall way off downstream. This pattern is notably consistent with observations seen in Section 5.6.

**Figure 7.5** Axial Profiles of Mixture Fraction and Temperature for Flame F
Figure 7.6 Axial Profiles of CH₄, O₂, H₂O and CO₂ Species Mass Fraction for Flame F
Figure 7.7  Axial Profiles of CO, OH, H₂ and NO Species Mass Fraction for Flame F
7.5 Flame F Radial Profiles

As with the Flame D results, analysis of the radial profiles for scalars at different downstream distances is necessary to evaluate how well the ODT-LES model predicts combustion behavior amidst the turbulent flow field. Once again the radial plots of scalars within the Flame F simulation are comparable to those seen in Flame D with similar discrepancies in and out of the flame regions. Figure 7.8 through Figure 7.17 show the radial profiles of transported scalars along with dependent scalars calculate through the LES closure tables. In Figure 7.8, the mixture fraction appears to align well with experimental results, with the exception of the area around $x/d=30$ where it is under predicted at the centerline. This would indicate that the scalar mixing is over-stated in this flame active region between $x/d=15$ and $x/d=45$. In contrast, the predicted temperature seen in Figure 7.9 is over predicted in the beginning stages of this region ($x/d=15$), but levels off to align with experimental values further downstream. This trend would indicate that while the scalar mixing is slightly overstated in these regions, prediction of extinction is still accomplished.

For the most part the predictions for secondary scalars is more accurate than those seen in the Flame D results, but similar issues remain. In Figure 7.10 and Figure 7.11, the fuel and oxidizer predictions are more accurate leading up to the active flame regions, but they tend to vary more significantly downstream. In contrast, predictions of saturated combustion products in Figure 7.12 and Figure 7.13 are overstated in the beginning stages of the flame region ($x/d=15$), but move closer to experimental data at the flame tip and beyond. The prediction of combustion radicals are also overstated in beginning stages of the flame region at $x/d=15$. Shown in Figure 7.14 through Figure 7.16, these scalars are reasonably accurate at $x/d=30$ and $x/d=45$, but they diverge positively or negatively up or
downstream depending on the variable. Interestingly, the predictions for CO and H$_2$
demonstrate similar patterns, which would indicate that the reaction mechanism used
contains strong correlations between the two scalars. Finally, the NO predictions appear to
be two part. In the areas nearest to the flame tip ($x/d=30$ and $x/d=45$), they are more
accurately predicted, while in the areas outside the flame zone, they are either dramatically
overstated ($x/d=2$ and $x/d=15$) or they are understated ($x/d=60$ and $x/d=75$).
Figure 7.8 Radial profiles of mixture fraction at downstream distances of $x/d=2, 15, 30, 45$ and 60
Figure 7.9 Radial profiles of temperature at downstream distances of \( \frac{x}{d} = 2, 15, 30, 45 \) and 60
Figure 7.10  Radial profiles of CH₄ mass fraction at downstream distances of x/d=2, 15, 30, 45 and 60
Figure 7.11 Radial profiles of $O_2$ mass fraction at downstream distances of $x/d = 2, 15, 30, 45$ and $60$
Figure 7.12 Radial profiles of $\text{H}_2\text{O}$ mass fraction at downstream distances of $x/d=2$, 15, 30, 45 and 60.
Figure 7.13 Radial profiles of CO$_2$ mass fraction at downstream distances of $x/d$=2, 15, 30, 45 and 60
Figure 7.14 Radial profiles of OH mass fraction at downstream distances of $x/d=2, 15, 30, 45$ and $60$
Figure 7.15  Radial profiles of CO mass fraction at downstream distances of $x/d=2$, 15, 30, 45 and 60
Figure 7.16  Radial profiles of $\text{H}_2$ mass fraction at downstream distances of $x/d=2, 15, 30, 45$ and $60$.
Radial Profile of $Y_{NO}$ – Flame F

Figure 7.17  Radial profiles of NO mass fraction at downstream distances of $x/d=2, 15, 30, 45$ and $60$
7.6 Flame F – State-Space

A good way to explain much of the behavior seen with secondary scalars as described in Sections 7.4 and 7.5 is to analyze plots of these variables in the mixture fraction state-space. Figure 7.18 through Figure 7.25 show each of the secondary scalars included in Sections 7.4 and 7.5 plotted as a function of mixture fraction. In all cases, the conditioned scalars match experimental results pretty well in the $x/d=30$ to $x/d=45$ range, but show some discrepancies in the other locations. The region between $x/d=30$ and $x/d=45$ is where the flame is well established, having the stoichiometric mixture fraction approaching the centerline. Notably, predictions of H$_2$ and NO in the $x/d=30$ plots are overstated in the area around the flame, which is also the region where a moderate amount of extinction is observed in Section 7.3. While other factors may be involved this shortfall is more likely due to the reaction mechanism used in the ODT simulations. As stated in Section 5.5 the reaction mechanism used in the ODT simulation to generate statistics has a limited ability to model NOx formation. That being the case, the pattern and data trends have more focus in this analysis. Looking at the plots for the position at $x/d=15$, it appears that the LES-ODT model is driving the reaction closer to completion than experiments. Predicted values for the fuel and oxidizer are lower than those from experiments, and the saturated combustion products are higher in conjunction. Likewise, the radical species are much higher than expected, which would imply that the model is predicting a less complete reaction during this stage. This, too, could be in part due to the reaction mechanism, but it could also be explained as a characteristic of how the model deals with this highly strained region of the flow. If we analyze Figure 7.9 in light of this statement, it is clear that the LES-ODT model is slightly
delayed in its representation of the quenching needed to contain the reaction in this portion of the flame.

With the exception of the fuel and oxidizer, all the species show elevated levels for around the stoichiometric mixture fraction in the $x/d=15$ region. This condition is consistent with what is observed in similar plots for Flame D, but is more pervasive in that all the species are affected. Similar to the arguments explaining errors in the Flame D results, the two more likely contributions to the error are the model sensitivity to state space errors and the shortcoming resulting from the handling of the learned KDFs for the higher variance regions. While the KDFs for mixture fraction in Figure 5.16 are better representations for the Flame F distributions in Section 4.1, the additional noise and unnatural modes present more of a challenge with the Flame F distributions. Issues with predicting scalar distributions in the $x/d=15$ region are evidence that the shortcomings mentioned in Section 5.8 result in KDFs that are less effective than desired. Once again, additional research examining the details of these distributions would be valuable.
Figure 7.18 Comparisons of conditional mean CH$_4$ species mass fraction in state-space at $x/d=7.5, 15, 30, 45, 60$ and 75 for Flame F. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow” is conditioned on $Z$. 
Figure 7.19 Comparisons of conditional mean O₂ species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame F. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow” is conditioned on $Z$. 
Figure 7.20 Comparisons of conditional mean H$_2$O species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame F. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow” is conditioned on $Z$. 
Figure 7.21 Comparisons of conditional mean CO$_2$ species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame F. Note that “LES-ODT” is conditioned on $\bar{Z}$, and “Barlow” is conditioned on $Z$. 
Figure 7.22 Comparisons of conditional mean OH species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame F. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow” is conditioned on $Z$. 
Figure 7.23 Comparisons of conditional mean CO species mass fraction in state-space at $x/d=7.5$, 15, 30, 45, 60 and 75 for Flame F. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow” is conditioned on $Z$. 
Figure 7.24 Comparisons of conditional mean H₂ species mass fraction in state-space at \(x/d = 7.5, 15, 30, 45, 60\) and 75 for Flame F. Note that “LES-ODT” is conditioned on \(\bar{Z}\), and “Barlow” is conditioned on \(Z\).
Figure 7.25 Comparisons of conditional mean NO species mass fraction in state-space at $x/d=7.5, 15, 30, 45, 60$ and $75$ for Flame F. Note that “LES-ODT” is conditioned on $\tilde{Z}$, and “Barlow” is conditioned on $Z$. 
7.7 Variance and Scalar Dissipation

One way to determine the effects of turbulence on transported scalars is to analyze the fluctuations and the dissipation. While LES closure does not rely the scalar dissipation rate, it is a good expression to evaluate for analysis and comparison. The scalar dissipation is defined as the square of the scalar gradient, which provides a high level view of scalar changes within a small region of the flow.

\[ \tilde{\chi} = 2D|\nabla \tilde{Z}|^2 \]  

(7.1)

Obtaining a filtered scalar dissipation from unfiltered (resolved) mixture fraction is difficult because of the convolution of \(|\nabla Z|^2\), thus many times it is modeled from other filtered terms. In the context of LES, the filtered scalar dissipation can be approximated from the magnitude of the square of the filtered mixture fraction, as seen in Eq. (7.1), or it can be modeled algebraically using the scalar variance.

\[ \tilde{\chi} = C_{\chi} \frac{\varepsilon}{k} \overline{Z \tilde{Z}} \]  

(7.2)

Figure 7.26 shows plots of the approximated version of \( \tilde{\chi} \) as well as the modeled version, \( C_{\chi} \frac{\varepsilon}{k} \overline{Z \tilde{Z}} \). The two different curves appear to be within good agreement of each other, reaffirming that they are interchangeable with regards to measuring the effects of turbulence in transported scalars. Consequently, levels of \( \tilde{\chi} \) from Eq. (7.1) are part of the discussion of local-extinction within the turbulent Flame F seen in the next section.
As mentioned previously, determining the best mechanism to evaluate, capture, and show evidence of local extinction and re-ignition tends to vary between research efforts. The previous sections of this chapter examine the scalar profiles, conditional statistics and the
scalar fluctuations for Flame F. Each set of results exhibits similarities with the experiments, but these comparisons alone don’t directly indicate the evidence of extinction and/or re-ignition. To expand this effort, contour plots of $Y_{\text{OH}}$, $Y_{\text{CO}}$ and $\tilde{x}$ are added and analyzed to better understand this combustion phenomenon. If observations from Section 5.6 are considered, the OH concentrations are expected to be highest on the front side of the flame where the temperature has yet to reach the equilibrium flame temperature. (Pettit, Coriton, Gomez, & Kempf, 2010) confirms this expectation with observations affirming that OH is a key property to identifying the location of the flame. Combining this information with the observation that higher concentrations of OH seem to be co-located with increased temperatures validates the usage of OH concentration levels to determine key aspects of non-premixed flames.

Figure 7.27 illustrates the spatial contour of OH species mass fraction alongside the corresponding temperature contour. Two observations are notable from this view. First, higher levels of temperature do coincide with elevated levels of OH concentrations. This feature is consistent with other aspects of this research as well as information from outside sources. Next, the flame in Figure 7.27 shows several examples where OH levels and temperature are reduced and then increased, which is consistent with the description of extinction and re-ignition. Figure 7.28 demonstrates the same phenomenon, but the results are more difficult to assess. CO concentration levels appear to be higher on the fuel rich side of the flame, and as seen in Figure 7.28, higher CO levels are more predominant in the latter portions where the flame is less extinguished. Finally, Figure 7.29 shows the levels of $\tilde{x}$ alongside the temperature. $\tilde{x}$ levels also appear to be highest on the fuel rich side of the flame, and they tend to be co-located with areas exhibiting extinction. As expected, higher levels of $\tilde{x}$ point to areas
of the flow that are more highly strained, thus causing the flame to be quenched. Each of these plots illustrate that the LES-ODT closure model provides good examples of extinction and re-ignition when simulating Flame F.

**Figure 7.27** OH species mass fraction contour plot on 2D centerline cross section for Flame F. The greyscale line shows the stoichiometric mixture fraction, and the light blue line is the outline of the flame.
Figure 7.28 CO species mass fraction contour plot on 2D centerline cross section for Flame F. The greyscale line shows the stoichiometric mixture fraction, and the light blue line is the outline of the flame.
Figure 7.29 $\chi$ contour plot on 2D centerline cross section for Flame F. The greyscale line shows the stoichiometric mixture fraction, and the light blue line is the outline of the flame.
8 Conclusion and Remarks on ODT-LES Model Potential

8.1 Introduction

A new method for tabulated LES closure has been investigated using stand-alone ODT simulations, combined with KDF, to provide both the conditional statistics and joint scalar distributions exclusively from data resulting from ODT realizations. A key aspect of this type of model is the creation of scalar FDFs for mixture fraction and temperature based on data collected from ODT simulations. These FDFs are enhanced using a kernel density estimator to create smooth distributions that track closely to the sample data. Sub-grid scalar values from the same data sets provide conditional statistics. Combined with the learned FDFs, these statistics are needed for LES closure for filtered density and unclosed source terms. Filtered species mass fractions are also resolved with this method in post processing. The ODT originated LES closure has been validated using an LES simulation of the Sandia Flames D and F. With these simulations, the model performed well enough to demonstrate many of the flame characteristics of interest. Of high importance is the ability to predict and show evidence of extinction and later re-ignition. These result have also been demonstrated and discussed.

8.2 Model Performance and Accuracy

From the discussion in Chapter 6 and 7, the accuracy of the LES-ODT closure model operates within an acceptable error margin, providing results that are matched reasonably well with experimental data. This statement of accuracy is true for both the explicitly transported variables such as temperature and mixture fraction as well as the secondary dependent variables such as species mixture fraction. The closure model input into a
transported variable is one of many contributions affecting its evolution. The dependent variables are calculated directly using the closure tables, so they are dependent solely on the contents of the table and the current state of the system. Thus, there are two different situations that affect the results for these scalars: the structure of the raw input fed into the tables, and the details of the distributions associated with selected variance ranges. A large issue encountered when constructing the closure tables is how to deal with sections of the state-space that do not have sample data. ODT simulations are excellent at providing sample data for conditions which match the simulation at hand; however, there is still information missing in required portions of the solution. As mentioned in Section 6.7, some of the errors seen in state-space plots of species mass fractions are likely to be the result of high sensitivity to error within the closure model. The completeness and accuracy of data outside the expected scalar data path directly affects the sensitivity of the model. The challenge, therefore, is how to provide data for a closure table used within an LES simulation that requires information from outside the known portions of the state-space. With the model studied here this gap is filled by merging cold flow boundary data in the regions that aren’t seen in the ODT domain. Unfortunately, merging cold flow boundary data with reacting flame data can result in regions of uncertainty or unwanted noise. Methods by which these anomalies are eliminated are worth considering and would be a significant improvement in the prediction of secondary scalars.

The code used to perform the ODT simulations is a single threaded non-parallelized Fortran program that is designed to write to a single data file. With a little organization and creative application, the code can be run in a highly parallelized fashion. The data is segmented by pointing groups of program instances to different files, and each of the
program instances are given a unique seed value based on instance and segment. The processes in each segment are automatically synchronized because they are appending to a shared file which does not have any particular order. The post processing of these segments, however, is more cumbersome to parallelize. In this step, the data in the unordered segment files are split into two groups. One group is re-written to another un-ordered list which contains the vectors needed to build the FDFs. The other is collated into a sorted list of vectors needed for the instantaneous values. Unfortunately, adding data to the sorted list of vectors in a parallel fashion is more complicated, therefore it was not implemented. As a result this portion of the pre-processing of the ODT generated statistics creates a huge bottleneck in the closure table construction process. One big improvement that would be valuable in later studies is the parallelization of the vector containing the collated instantaneous data. Parallelizing the accumulation step could save several days in the process of constructing the closure table.

8.3 Challenges and Drawbacks

While the LES-ODT method introduced in this study provides benefits over existing methods, several challenges still remain. As mentioned above having a better representation of the conditional statistics in the state space regions not observed from ODT simulation will improve the closure table’s sensitivity to fluctuations in the state space. Next, issues regarding the handling of learned KDFs which are highlighted in Section 5.8 represent a key aspect of the model that should be improved. It is important that the learned KDFs be representative of turbulent flame scalars; however, the error related overhead when preparing the data may result in predictions that are less accurate than desirable. Thus, a balance must be struck between the
value of a representative KDF and errors introduced through data smoothing and noise elimination. Lastly, the selection of distribution variance ranges requires optimization. Section 4.5 illustrates the process for selecting the best set of parameters required to construct the filter density functions. While the graphical tools used to assist in the selection of these parameters proved helpful, manual selection may not be ideal. The selection process can be accelerated and more accurate by using numerical categorization techniques, but the final decision is still in the hands of the system designer. These selections are essentially an empirical set of parameters applied to render the desired distributions, but a solution which is constructed without empirical parameters is a better choice. An investment in determining best case distribution parameters without human input is warranted.

On a different note, while OpenFOAM proved to be a good choice for this research, one of OpenFOAM’s biggest limitation is the lack of tested, validated, non-Cartesian coordinate systems. Typical 3D solutions for an axial jet problem use either spherical or cylindrical coordinate systems. These choices eliminate the errors associated with mapping circular boundary conditions with quadrilateral coordinates. Implementation of the velocity boundary described in Section 6.2 requires a bit of creative data manipulation in order to attach the proper velocity magnitude to the associated field location. With a curvilinear coordinate system these boundaries are much simpler to implement, and more accurately represent the actual boundary. Similar issues exist with the many post processing applications and the gathering of field data for analysis. Thus, an investment in developing good solutions for cylindrical and spherical coordinate systems for OpenFOAM would be a great addition to an already good choice of CFD packages.
8.4 ODT-LES Model Variations

In this study, ODT is used to construct multivariate tables which resolve the unclosed filtered non-linear scalar terms in an LES transport equation. This approach provides a simple mechanism to complete the LES solution while maintaining a good degree of accuracy. Even though the examples in this study focus on non-premixed jet flames, this ODT closure method and the artifacts rendered during the model construction process can be applied to a variety of other turbulent combustion problems. Where data from ODT realizations are needed to build distributions for the temperature and mixture fraction, a similar method can be used to build distributions for pre-mixed progress variables or a reduced set of scalars representing the state of the system. The progress variable is needed to define the chemical state in a turbulent pre-mixed flame, and the reduced set of scalars are part of applications focused on principle component analysis.

Alternatively, an ODT realization can be applied to generate artifacts containing distributions concurrent with conditional statistics. These methods build multi-variate regression tables from the raw data without the extra step of extracting and building the necessary scalar distributions. One such method uses artificial neural networks (ANN) to replicate a complex non-linear regression function with a network of switched linear functions. Each function is switched on or off with a coefficient, and the coefficients are learned from a given set of correlated data. In the LES-ODT tabulation method statistical distributions of state scalars are explicitly extracted from the data using correlated vectors; however, with the ANN the statistical distributions are implicitly determined via the coefficients within the network. Several studies have shown good success with using ANNs to reduce the overhead of dealing with complex reaction mechanisms, but most of these focus on the deterministic
nature of the reaction mechanism (Sen & Menon, 2010). More recently (Mirgolbabaei & Echekki, 2013) applied the ANN method to a unique approach to dealing with the ODT transport equations used in an ODT-LES solution. Instead of solving the entire set of species transport equations in a coupled LES-ODT problem, a set of key mass fractions are considered as the principal components extracted from the eigenvectors. This application requires a complex algorithm to determine the source terms on the right hand side of the ODT transport equations. The ANN regression method proved to work quite well in cases where the source terms were defined as a network parameterized by the principal components. The networks were trained using a stand-alone ODT much like that described in Chapter 3, but the data was later needed to determine the source terms for the required principal components. This research omits analysis of the statistical distributions related to the large scale flow, but it is a good example of capturing a complex problem with a set of more simplistic elements.

While ANN provides a lightweight solution to the non-linear regression problem represented in the multi-variate dataset, this same information can be represented with a multi-dimensional table much like the closure table described in Section 4.8. The data collection process would use the filtering function within ODT to store filtered datasets, and the table construction would be similar to much of pre-processing steps described in Chapter 4. The biggest difference with this method from that described in Chapter 4 is that tabulated data is spatially filtered within the ODT domain rather than being filtered in state-space. The closure table indices then are determined by corresponding filtered state variables and associated variances. Finally, because the composition of the tabulated closure model is exactly the same regardless of whether the scalar distributions are explicitly defined or implicitly included, the LES implementation is equivalent. Thus, a model which is constructed using implied
distributions can be validated with the same LES code as that used in Chapter 6. The biggest drawback to this approach is overcoming the challenges associated with completing the overall view within state-space. Without an integration step, the interpolation process must be more advanced to better determine the missing data.

8.5 Necessary Improvements

While the LES-ODT closure model operates reasonably well in the Sandia Flames, several improvements could be investigated for better applicability and accuracy. First, due to the number of data points and dimensionality, the size of the closure table is limited to a relatively small number of variance indices. Expanding this limitation to include a more granular set of scalar variances would conceivably enhance the transitions from each of the levels of turbulence and capture more of the desired sub-grid behavior. Having a limited number of points makes selecting the boundaries more difficult and forces the data to be categorized in disproportionate segments, thus a large number of ranges are desired. Unfortunately, having a more granular set of indices requires additional samples, thus a larger number of ODT realizations are required.

As mentioned previously, adjustments resulting in cleaner KDFs which contain only information that is necessary to close the turbulent combustion solution have immediate and long term value. The different approaches to improving KDFs that are described in Section 5.8 could potentially require a significant effort. In order to streamline the work, distributions that can be better compared side by side with experimental data are necessary. A preliminary improvement to this research would be the assembly and representation of learned KDFs such that they can be evaluated better in side-by-side comparisons with experimental PDFs. Once
these types of comparisons are supported, improvements with the handling of the ODT distributions can be better evaluated along with the final results seen in LES simulations.

One of the many assumptions made when constructing the models for this study is the applicability of the 1-D filter used to construct the FDF statistics. As discussed in Chapter 3, the statistical characteristics of an axisymmetric turbulent jet reinforce the assumption that a 1D view can capture the statistics necessary to analyze distributions associated with filtered scalars. In order to expand the capabilities of the LES-ODT closure model to problem domains that do not carry the same assumptions as the axisymmetric jet, an extra dimension is more likely to be needed to capture the filter distributions found in scalar statistics. This additional dimension can either be added by making the ODT solution a 2D problem, or by filtering the solution in the streamwise direction through time. Filtering downstream requires keeping track of multiple copies of the ODT solution, thus adding additional overhead and complexity, but the concept is a very feasible addition. Simple tests may be required to determine if expanding to a 2D filter is of value or not.

8.6 Future Research and Suggested topics

Based on several of the conclusions drawn above, several topics deserve special attention and future research investment. First and foremost, the use of ODT to extract scalar distributions matching select problem domains is a practice that is not necessarily limited to LES closure as described here. The process can be applied to other LES-ODT problems, and can even be expanded for use with different closure methods. For any closure method that requires an input distribution to construct the functional definition of a filtered quantity, ODT provided statistics are excellent for this type of artifact. There is potential for usage of ODT
generated statistics in methods such as the flamelet model or CMC closure. Thus, in addition to research applying LES closure to other types of problems, the methods used to extract distributions from ODT generated statistics should be considered in other applications that require state-space variables.

Even though the practice of using extracted distributions shows great potential with both LES-ODT as well as other state-based closure models, methods relying on implied distributions can be much more efficient and compact. A direct extension of this research is the application of closure tables generated from quantities filtered directly in the ODT domain. The basic hypothesis of this proposed research is that a closure table filtered in the ODT domain is equivalent to a closure table filtered through integration of ODT statistics. This validation could use much of the work herein, extending the table construction method to include filtered quantities. Furthermore, results in the present research can be incorporated into comparisons between model changes and experimental results. If using implied distributions proves to be possible, another extension to this research would be to construct a more functional closure artifact using numerical learning techniques such as the ANN. A neural network defined and learned for each of the filtered variables would replace the tabulated closure. The more complex aspect of this extension is the parameter selections and the process by which each network is learned from the filtered ODT statistics.

Each of these proposed research topics are extensions to the work performed thus far, so much of the codes and utilities used here can be expanded and extended to support the next stage of development. One aspect of validation that has been omitted from this research is the comparison of results between distribution parameters. Isolating just the changes in the distributions needed to construct the closure tables and comparing the effects of these changes
in the results would be a great addition to promoting the application of learned distributions from ODT simulations. The stages could include first comparisons between results similar to those in this research with results produced from using the $\beta$-PDF. Then, changes in how the variances are selected and determined can be evaluated. Finally, changes or additions in the filtering process can be tested. Having the ability to compare changes in the distributions alone would clarify the importance and understanding of the need to pick distributions that best match the problem in question.

In summary, the LES-ODT closure model exposes some very important aspects of ODT, pointing mainly to the untapped potential hidden within what appears to be a simple solution to a complex problem. When equivalent amounts of information from a 3D simulation are possible in a 1D simulation, a much more efficient and usable solution to complex problems is possible. Having the ability to build useful distribution for use in LES closure from ODT simulations is a good addition to the already available set of ODT applications. This research has shown that scalar distributions can be extracted from ODT simulations, and that by using kernel density functions these distributions can be made robust enough for use in LES closure. Even though these methods and distributions aren’t expected to replace all FDF options, they are a good addition to available choices.
REFERENCES


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APPENDICES
Appendix A – LES solver using OpenFOAM

A1. Why Choose OpenFOAM

When choosing a CFD package to perform turbulent combustion research several factors must be considered: cost, extensibility, performance and availability. Considering this research was essentially unfunded, cost is a primary factor. However, the need to implement a new closure model and manage control of boundary conditions also places a high degree of importance on the extensibility of the product. Finally, improved performance and high availability are certainly pluses. Any one of the highly known CFD packages such as Ansys’s Fluent, CFD Software’s Flow3D or Exa’s PowerFlow would be an excellent choice for analysis considering performance and usability; however, each of these product are cost prohibitive so other alternatives are more attractive. While there are a slew of available free and open-source CFD software available, many are designed for specific types of problems or are limited to simple solutions. OpenFOAM on the other hand has the expansive capabilities of the commercial products without the large monetary cost. Instead, the cost when working with OpenFOAM is manifested in the implementation details. Either way, without cash funding, the implementation overhead is worth the investment.

OpenFOAM is a C++ based open-source product which offers a vast number of implementation options with a high degree of complexity. While there are many tutorials and examples, implementation beyond standard formats requires a large investment in education and experience. This investment is deemed a decent ROI in both understanding and experience. Several research efforts have used OpenFOAM beyond the simple educational examples (Ding, Wang, & Lu, 2014), and with each release the OpenFOAM product is gaining
more attention and users. OpenFOAM is distributed by OpenCFD which also provides a commercial version that includes services and support. So whether the user is a PhD student or a large corporation such as Volkswagen, OpenFOAM offers the performance and flexibility that can fulfill the needs of many applications. For this research OpenFOAM has been a good choice considering the implementation details and the performance characteristics. The product has been installed and used in conjunction with other resources available within the HPC community at NCSU. Within the timeframe of this research, the studies have been through 3 different OpenFOAM releases. The first implementation used version 1.7.0, the preliminary results were created using version 2.1.1, and the final results were produced with version 2.3.1. With each upgrade, the custom implementation of the closure model requires updates to adapt to associated changes with dependent models. The remaining sections of Appendix A describe the infrastructure and content of the LES solution which is implemented via OpenFOAM.

A2. “mixtureFractionFOAM”

“mixtureFractionFOAM” is the custom application implemented to perform the LES simulation used in this dissertation. The code is loosely based on the implementation of the fireFOAM product which is managed by FM Global (Ding, Wang, & Lu, 2014). The two codes are similar in their use of the PIMPLE algorithm to solve the pressure equation using a predicted velocity. They also share similar numerical methods for convective terms and integrations common among many OpenFOAM products. The biggest differences lie in the scalar transport equations and the implementation of the source terms. mixtureFractionFOAM does not solve the conservation of mass equation. Instead, it calculates the density using the
LES-ODT closure model, and integrates the result into the remaining transport equations. Both the density and the source equations use custom classes to load and manage the multi-dimensional closure tables outlined in Section 4.8. These classes also rely on the scalar variances which are solved using independent transport equations. As the title indicates, in addition to the energy conservation equation, the solution is defined by the transport of the mixture fraction. This transported solution variable determines the other transport variables defined via a fuel stream, an oxidizer stream and the products. Note that these other variables are only used for calculating thermochemical properties, and they are not included in the filtered density or chemical source term.

### A3. PIMPLE Method for solving Pressure and Velocity

One of the more significant challenges when solving the momentum equation is determining the pressure field. The pressure gradient shows up on the right hand side of the momentum transport equation, but the pressure field is actually dependent on the momentum. Patankar’s method involves solving for the pressure by splitting it into a guessed value plus a correction; solving for the velocity using the guessed pressure; then determining the final pressure using the velocity (Patankar, 1980).

\[ p = p^* + p' \] (9.1)

Initially, the value \( p^* \) is a just a guess, but as the solution progresses, the guessed value for each iteration is the previous value. Likewise, the velocity is split into a guessed value plus a correction.

\[ u_j = u_j^* + u_j' \] (9.2)
The momentum equation is first used to solve for an estimated velocity \( u_j^* \) using the guessed pressure.

\[
\frac{\partial \tilde{\rho} \tilde{u}_j^*}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{u}_j^*}{\partial x_i} = \frac{\partial}{\partial x_i} \left( (2\nu_T) \tilde{S}_{ij} \right) - \frac{\partial \tilde{p}^*}{\partial x_j}
\]  

(9.3)

With the estimated velocity \( \tilde{u}_j^* \), the pressure correction \( p' \) is solved using Poisson’s equation.

\[
\Delta p' = \frac{1}{\Delta t} \left[ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_j^*}{\partial x_j} \right]
\]  

(9.4)

Once the corrected pressure is calculated, the velocity is updated with the final value.

\[
u_j = u_j^* + \frac{\partial \tilde{p}'}{\partial x_j}
\]  

(9.5)

The process then starts all over again using the corrected pressure as the next guess.

Further refinements to this method have been added to improve convergence and better calculation of the final pressure field. One improved method is called pressure implicit splitting operators (PISO). With the PISO method additional non-linear operators are added to better correct the predicted pressure which improves the handling of grid skewness and boundaries (Issa, 1985). These additions also improve convergence without a large number of iterations. Reducing or eliminating the need to iterate is important because the iteration process requires the solution to reach an incompressible steady state condition in order to be accurate.

For problems requiring variable density and non-equilibrium, the SIMPLE procedure without the additional operators is not sufficient; however, for large scale solution the PISO time step may be too restrictive. These restrictions lead to the development of the PIMPLE algorithm which is essentially an iterative variation of the PISO method.
The main objective with the pressure implicit algorithm is to ensure solution convergence without a highly restrictive time step. The SIMPLE algorithm is sometimes slow to converge when solving the pressure equation. This slowness is due to the errors generated due to not solving part of the correction terms. The SIMPLE algorithm splits the correction terms into two parts but then promptly neglects the second portion.

\[ U' = U'_1 + U'_2; \quad U'_2 \ll U'_1 \]

PISO accounts for this by adding a correction step to solve for \( U'_2 \) term. The momentum is then solved a second time using the additional correction term. This addition converges faster and is more accurate; however, the process requires a much smaller time step. The improved convergence comes at the cost of a smaller time step. To counter this issue the PIMPLE method uses factors and coefficients to balance the solution between the ideal time step and a faster convergence in the correction step. Instead of predetermining a “smaller” time step to satisfy the needs of the PISO algorithm, the PIMPLE algorithm iterates a variable number of correction steps to more accurately go from one time step to the next. In the OpenFOAM implementation, the set maximum number of iterations per time step provides variability to fit the needs of many different solutions.

A4. LES Density pressure dependence

In order to complete the system, the density is calculated without solving the conservation of mass. While the closure method based on tabulation does not explicitly include a pressure, the result should have the same basic requirements as when solving the filtered equation of state. This constraint implies that the local function to determine the density must also include the pressure as a means to match the state variables minimizing discontinuities.
A simple approach to solving the density without a conservation equation while also including the pressure is to solve an equation of state for the density which is a function of the pressure, the temperature and the chemical state. With the solution relying on a filtered density, which is also dependent on filtered quantities, it is best to relate the density as a function of the filtered pressure, the Favre filtered mixture fraction, and the Favre filtered Temperature. A closure method based on ODT data must then account for the difference in the ODT pressure and the LES pressure. A constant pressure is assumed when building the ODT density, so the LES closure $\rho_{cts}$ must apply ratios of pressure and density to remove the pressure dependence from the closure table.

$$\bar{\rho} = \frac{\bar{p}}{p_{const}} \rho_{cts}(p_{const}, \bar{\bar{Z}}, \bar{T})$$

(9.6)

In each iteration within the LES solver, the density field is calculated using the guessed pressure, and, then, again using the final pressure. This coupling between the density, the guessed and final pressure, and ultimately the momentum transport is a key element connecting the turbulence with the energy changes within the flow field, attempting to keep the pressure and momentum consistent.

**A5. Boundary Conditions**

An important aspect of the LES solver used to simulate the TNF Sandia Flames is the method by which the boundary conditions are implemented. At the inlet the velocity accounts for turbulent conditions as well as the natural shape of a fluid injection into a free stream. The boundaries at the sides support entrainment while keeping the energy balance consistent. Finally, the exit boundary allows for turbulent fluctuations and changes in the pressure. In the
domain definition for the Sandia Flames, there are 5 different boundary fields defined: base, sides, outlet, fuelinlet and pilotinlet. The base represents the co-flow stream which is a set to a fixed velocity with no turbulent characteristics. The sides are defined using the “pressureInletOutletVelocity” boundary which is a mixed boundary condition where the exchange is determined by direction of the flow, which is driven by the pressure.

\[ au(x) + b \frac{\partial}{\partial x} u(x) = C \]  \hspace{1cm} (9.7)

\[ p_t = p_s + \frac{1}{2} \rho u^2 \]

The outlet boundary is a an “inletOutlet” condition which is the top half of the “pressureInletOutletBoundary” which is either a fixed value boundary when the flow is outbound or a zero gradient boundary when the flow in inbound.

Finally, the fuelinlet and pilotinlet boundaries are implemented using a custom mapped turbulent boundary. The map is defined using a spline function which defines the magnitude of the velocity based on the distance from the origin. The turbulent aspect of the boundary is created by adding fluctuations to the resulting boundary map during each time step. The implementation of this type of inlet boundary increases the effective turbulence with a parameterized factor \( \alpha \) that is included in the description of the velocity fluctuations. This approach is applied numerically to the data contained in \textbf{Table 5.3}, resulting in a time varying inlet velocity that can be adjusted.

\[ U(x, t) = (1 - \alpha)U_c(x) + \alpha U'(t) \]  \hspace{1cm} (9.8)

In Eq. (9.8), \( U_c \) and \( U'(t) \) are determined by the data in \textbf{Table 5.3}, and \( \alpha \) is a scaling factor needed to adjust the magnitude of the fluctuations. \( \alpha \) is increased for Flame F
simulation, as compared with Flame D. in order to also increase the likelihood of turbulent fluctuations in the inlet velocity.

**A6. Heat transfer and Radiation Methods**

Even though heat transfer and radiation are many times neglected in theoretical models, representing real world problems without capturing these effects can resulting in undesirable errors with regards to the energy conservation. Heat transfer is usually important in flows surrounded by walls such as combustion chambers or enclosed fires which not so much the case with a jet diffusion flame protruding into a free stream. However, in cases where soot formation is possible, the transfer of heat to the stream particles could become important. For this reason heat transferred to particles and free flowing surfaces is considered when constructing models for realistic combustion environments.

At high temperature thermal radiation is a very important phenomenon which cannot be neglected. The Stephen-Boltzmanns equation relates the heat radiated from an object to the temperature to the fourth power.

\[ P = e\sigma A (T^4 - T_{c}^{4}) \]  \hspace{1cm} (9.9)

If the difference between the flame temperature and the cold flow temperature is significant, then the result from eq. (9.9) cannot be neglected (Bejan, 1993). Unfortunately, because the area A is determined by the angle of incident among each of the emitters, solving this equation in a 3D domain can be quite complicated. The method for solving this equation within the OpenFOAM framework is called fvDOM. This class is a finite volume solution for eq. (9.9) using a discrete number of angles which are defined within a subdomain of the containing finite volume domain. Due to the potential for a large amount of computational
overhead the angles within the volume are limited to a smaller number creating a coarse
discretization. Even though the angular grid is coarse, the method is conservative and accounts
for all of the characteristics of radiation such as the scatter pattern, the transport media, and
surface properties. Thus, it is an effective method to account for radiation with a combustion
simulation.

In many non-premixed combustion problems, soot formation and destruction is of great
interest. Soot particles form as a result of a series of surface reactions due to containments in
the fuel. While these processes are typically neglected in experimental flames, they cannot be
neglected for realistic problems. Likewise, problems that include surfaces must account for
thermal and chemical processes at the interface. These processes can result in thermodynamic
effects that may lead to a phase change, modifying the composition of the solution. Even
though the phase changes and surface effects are not huge factors in the analysis of Sandia
Flames, they are included within the mixtureFractionFOAM code for completeness. Including
these effect keeps the solution generic such that it can be expanded to other problems later.

A7. Scalar Variance Transport Equations

The variance transport equation discussed in Section 2.8 requires three of the
included terms to be closed using algebraic expression or terms from the solution variables.
These expressions represent the sources and sinks associated with the scalar variance.

\[ \bar{\rho} D_T \left( \frac{\partial T}{\partial x_j} \right)^2 \] provides the effects associated with the scalar gradient; \[ \bar{T}' \omega_T \] provides the
changes associated with the fluctuations in the temperature source; and \[ \bar{\rho} \tau T'' \frac{\bar{\varepsilon}}{2k} \] provides
information associated with the dissipation of flow energy. \( \bar{\rho} D_T \left( \frac{\partial T}{\partial x_j} \right)^2 \) is calculated directly
because $\bar{\rho}$ and $\bar{T}$ are both readily available from the solution. The second term $T^r \omega_r$ is determined using the closure table which is described in Section 4.8. Finally, the term $T^{r2}$ is part of the solution, but $\frac{\bar{\varepsilon}}{2\bar{k}}$ requires special attention. While an algebraic model will work, the OpenFOAM turbulence model exposes expressions for both $\bar{\varepsilon}$ and $\bar{k}$. The OpenFOAM Smagorinsky LES Turbulent Model defines epsilon follows.

$$\bar{\varepsilon} = \frac{C_\varepsilon \bar{k}^{3/2}}{\Delta}$$ \hfill (9.10)

Substituting Eq. (9.10) into the expression $\frac{\bar{\varepsilon}}{2\bar{k}}$ yields an equation which is only a function of $k$ and $\Delta$.

$$\frac{\bar{\varepsilon}}{\bar{k}} = \frac{C_\varepsilon \bar{k}^{1/2}}{2\Delta}$$ \hfill (9.11)

The only remaining issue is how to handle $\Delta$. For the most part $\Delta$ does not inadvertently affect the variance; however, in regions close to the boundaries where the grid implies a much smaller $\Delta$ the variance can be artificially increased to differences in the LES grid. To combat this, a globally averaged $\Delta$ is used for Eq. (9.11) rather than the localized version.

A8. Calculation of Temperature from Conservative Enthalpy

Within the OpenFOAM LES framework, the temperature is a secondary variable which is dependent on the transported enthalpy. By considering the temperature as function of the enthalpy a cyclic dependency results due to the dependence of enthalpy on temperature.
\[ T = f(h_s(T, p)) \]  
(9.12)

This functional dependence is challenging to solve directly, thus a numerical iterative method must be applied. The Newton-Raphson method is an iterative method that can be used to find the roots of a non-linear zero valued function \( f(x) = 0 \) (Bird, 2010).

\[ x_{n+1} = x_n - \frac{f(x)}{f'(x)} \]  
(9.13)

This method can be applied to find the temperature corresponding to a given value of enthalpy by defining the function \( f(x) \) as the difference between the known value of enthalpy and the one corresponding to the dependent temperature.

\[ f(p, T) = h_s(T, p) - h_{s,n} = 0 \]  
(9.14)

The derivative of \( h_s(T, p) \) can also be represented as the specific heat at constant pressure \( C_p = \frac{dh_s}{dT} \), and when treating \( h_{s,n} \) as a constant in Eq. (9.14), the derivative of \( f(p, T) \) is simply the specific heat at constant pressure.

\[ f'(p, T) = C_p \]

Substituting these terms into Eq. (9.13) yields an iterative expression to solve for the temperature which corresponds to a given value of enthalpy.

\[ T_{n+1} = T_n - \frac{h_s(T, p) - h_{s,n}}{C_p(T, p)} \]  
(9.15)

Equation (9.15) is solved iteratively until \( (T_{n+1} - T_n) < T_{err} \), and the procedure is started each time with \( T_n = T_0 \) where \( T_0 \) is a reference temperature.
A9. Post Processing Analysis and Tools

OpenFOAM provides three main utilities to analyze solution results after a simulation is completed. Probes are used to gather data from specific points defined in the configuration files. Samples are collections of data gathered within defined regions. Finally, paraFoam is a full scale graphics utility which enables users to view solution results within a three-dimensional environment. The results discussed in Chapters 7 and 8 fall into three different categories: (a) time averaged spatial profiles, (b) conditional statistics, and (c) multi-dimensional contours. The time averaged axial profiles are the result of executing specified probes for each of the available time slices, followed by a time averaging procedure to determine the averaged value at each probe location. The probe operation is a standard OpenFOAM post processing routine, but the time averaging procedure is a custom C++ application to process the probe results. Radial profiles require an additional set of steps in order to accumulate the needed data. Each instantaneous profile is the result of cylindrical average at each of the radial locations specified. These results are then time averaged in a manner similar to the procedure used with the axial profiles. This multi-step procedure is performed for each of the designated axial locations. Conditional statistics are the result of a set of surface samples accumulated and re-organized by the conditioning variables (mixture fraction and/or temperature). Data is gathered over a set of time slices; however, the data is a collection, instead of an average like the other processes. Finally, the 2D contours are the result of a sample via a 2D slice. The paraView application is used to render the visual images.
Appendix B – MATLAB toolbox

B1. Introduction

When considering possible methods for performing complex algebraic functions, one of the more significant factors is accuracy. While the implementation cannot necessarily account for flaws in the methodology, MATLAB routines and functions have proven to be error free and generally easy to use. Likewise, for processes such as interpolation and distribution construction MATLAB has developed quite a reputation as a decent choice. As part of the research performed in this study the two functions needed that are not already built into the custom applications are the interpolation of the multivariate data and construction of distributions based on discrete one-dimensional curves. Instead of implementing these routines from scratch, efficiency was gained by performing these functions with scripts executed by MATLAB. Each script converts the available data into a format amenable to the MATLAB routines, and then the data is written back to a file in a format expected by the next step of the construction process.

B2. MATLAB Interpolation

In Figure 4.6 the artifacts from the pre-processing step are in two different formats. The raw state vectors are saved in a binary format where the distribution vectors are stored in a raw text format. Pre-processing the raw state vectors involves reading each vector instance and separating the fields into columns to be processed. Post processing step 3a which is illustrated in Eq. (4.6) is accomplished via the MATLAB function “scatteredInterpolant”. This function takes three unordered but correlated lists where the first two are the coordinates for
each known value in a 2D grid. The generated object then populates a 2D mesh with interpolated values at each of the data points. The script process is simple: read input vectors into correlated lists, generate mesh grid for the target table, run “scatteredInterpolate” routine to obtain functional representation of the data. Then with this function the interpolated values are saved to a new binary file. The “scatteredInterpolate” function can use one of the following interpolation methods: natural, nearest and linear. Nearest interpolation applies the value of the nearest known instance to the interpolation point. This type of interpolation isn’t very useful with continuous scalars because it generates jump discontinuities in the grid. Natural interpolation finds the natural neighbors which are defined via the Delauney triangulation, and then combines them via a proportionate weight scheme. Finally, linear combines the values of the 4 surrounding data points using weights which are proportional to the distance. After several experiments the linear scheme was found to render the smoother and more realistic results. Even though the linear interpolation is less accurate, the monotonic characteristic provides a more predictable set of data tables. In addition to interpolating the raw 2D samples from ODT realizations, the MATLAB interpolation functions are used to fill in the boundary samples that fill the outer regions of the ODT data.

### B3. MATLAB FDF Construction

Building the FDFs needed for integrating filtered variables is a two-step process that first uses the kernel density function to create a fitted curve followed by the “pdf” function which converts the fitted curve into a normalized pdf. The kernel density function is implemented within the “fitdist” function, which uses one of 4 different kernel functions: “normal”, box, triangle and epanechnikov. The kernel function selected is the K in Eq. (4.1)
which has shown to affect both the smoothness and the functional bias. “Normal” uses the normal or Gaussian distributions; “box” uses direct delta functions; “triangle” uses a pair of linear functions with opposite slopes; and “Epanechnikov” uses a set of quadratic functions with a negative derivative. Keeping in mind that a smooth distribution is most ideal, the “Epanechnikov” kernel has shown to yield the best results. Similar to the interpolation process, each kernel distribution is saved in a 2D table which is indexed by mean and variance values. Each distribution has a discrete number of points (R), and there are N x M distributions; thus, the distribution table is R x N x M points.

Appendix C – Additional Plots

C1. Sandia Flame D – Scalar Variance and Source Terms

Even though there are no available experimental datasets for comparison, plots of scalar variances are presented. Figure 8.1 shows the scalar variances of mixture fraction and temperature along with the source terms for temperature variance and enthalpy. In comparing the difference between the mixture fraction variance and the temperature variance it is evident that the source term plays a significant role in the associated behavior. This comparison is a good illustration of why algebraic models fall short when dealing with reactive scalars. The variances of reactive scalars are tightly coupled with the mechanisms that drive combustion as well as those that drive the turbulence. A single linear expression is incapable of capturing such an interdependent relationship, and thus these results highlight the importance of using transport equations with these types of variables. The radial profiles in Figure 8.2 and Figure
8.3 are not much different than would be expected. Both are highest closer to the burner tip, and both are elevated in regions of steep scalar gradients.

**Figure 8.1** Scalar Variances and additional source terms for Flame D
Figure 8.2 Radial profiles of $\overline{Z''Z''}$ with $\tilde{Z}$ at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame D.
Figure 8.3 Radial profiles of $\overline{T'/T'}$ with $\overline{T}$ at $r/d = 2, 15, 30, 45, 60$ and 75 for Flame D
C2. Sandia Flame F – Scalar Variance and Source Terms

Scalar Variances and source terms in Flame F are also presented. Shown in Figure 8.4, plots of axial profiles show similar features to those provided for Flame D, but there are several differences in the area from $x/d=10$ to $x/d=30$. First the variance levels for both mixture fraction and temperature are elevated, resulting in a different axial profile. Next the source term for the temperature variance has two different maxima: one at around $x/d=20$ and the other just before the flame tip around $x/d=40$. On the other hand, with the exception of subtle differences in shape and magnitude, the radial profiles in for Flame F, in Figure 8.5 and Figure 8.6, are similar also to Flame D. Further investigation of the differences in the axial plots versus the similarities in the radial plots may be necessary.
Figure 8.4  Axial profiles of Scalar Variances and source terms for Flame F
Figure 8.5 Radial profiles of $\overline{Z'Z''}$ and $\overline{Z}$ at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame F
Figure 8.6 Radial profiles of $\overline{T^mT^n}$ and $\overline{T}$ at $r/d = 2, 15, 30, 45, 60$ and $75$ for Flame F
Appendix D – Statistics and Turbulent Combustion

D1. Statistical Background

Due to the apparent randomness of turbulent flows statistical tools are very important to the study of turbulence. These tools provide a means of identifying and characterizing the correlations and data distributions which support the many methods scientists use to describe this phenomenon. A probability distribution function (PDF) is a continuous positive function that can represent the numerical possibility that an event or value is present within a process or domain. This statistical tool has become highly used in turbulence models due to the stochastic nature of turbulence and the consistent properties of a PDF. For the most part, PDFs predict scalar quantities within a turbulent flow field, but some applications require a more complex definition of PDFs, encompassing joint probabilities of all the factors contributing to the system state. Whether solving the complex state problem or predicting scalar quantities, PDFs are valuable tools in the study of turbulence. The discussion which follows provides the key characteristics making the PDF an essential tool in studying turbulent combustion problems.

A PDF has two main properties that make it attractive as a statistical tool: the value is always non-negative and the sum of all the values equals unity.

\[ P(x) \geq 0 \]

\[ \int_{-\infty}^{\infty} P(x)dx = 1 \quad (9.16) \]

The first property ensures the absence of negative terms, and the second property states that the results from the distribution are normalized. Normalization facilitates integrating terms
within a domain to capture statistical moments. In most instances the first and second moments are necessary inputs for RANS and LES closure methods. For instance, the first moment of a variable \( \varphi \) which is a function of an independent \( \eta \) variable can be calculated from the integral of the product of the PDF and the fluctuating value over the range of \( \eta \).

\[
\langle \varphi(\eta) \rangle = \int_{-\infty}^{\infty} \varphi(\eta) P(\eta) d\eta
\]  

(9.17)

Whether the mean is defined using the above formulation or via an ensemble average, it is considered equivalent within the RANS formulation. For this reason knowing the PDF of RANS variables is essential when requiring first and second moments. Joint PDFs are used in cases that require multiple variables to describe the state of the system. Assuming statistically independent variables, the first moment of a multivariate quantity can be found by simply combining the PDFs as mentioned above.

\[
\langle \varphi(\eta, \zeta) \rangle = \iint_{-\infty}^{\infty} \varphi(\eta, \zeta) P(\eta) P(\zeta) d\eta d\zeta
\]  

(9.18)

The challenge with using a PDF to represent a turbulent scalar is the selection of functions which best represent the physics involved in the target study. Ideally, models should use a PDF which best represents the actual statistics within the studied domain without adding additional numerical errors. This representation can be accomplished by either selecting appropriate empirical distributions or by performing statistical analysis on available data. Data needed in statistical analysis can be obtained from experiments or from highly resolved simulations. Direct analysis of data sets requires organization and consistency, but using a prescribed PDF requires complete understanding of the physics in question. Empirical functions may be simpler, but they may also be limited to certain problem domains and
turbulent character. Historically, the $\beta$-PDF has been chosen to represent the distribution of a scalar quantity within a turbulent flow field. While this may be sufficient for non-reactive scalars, the function tends to fall short where reactive scalars exhibiting bimodal characteristics are present in regions of extinction and re-ignition (Ihme & Pitsch, 2008). For this reason distributions based on real statistics should be favored over prescribed distributions which tend to be symmetrical.

Some solutions such as the PDF transport method require the joint PDF be correlated, but many applications assume that the PDF’s are statistically independent. In cases where the scalars considered are not directly correlated, statistical independence can simplify the solution significantly, but some variables are inherently correlated so the independence is not warranted. According to Bayes Theorem, a conditional PDF can be obtained by simply removing the contribution of the conditional term (Alpaydin, 2010).

$$P(A|B) = \frac{P(A, B)}{P(B)}$$

(9.19)

It is clear from this description that having statistically independent variables $P(A|B) = P(A)$ leads to the joint PDF being described as $P(A, B) = P(A)P(B)$. In general, state defining scalars such as temperature and mixture fraction are assumed to be independent, so this relation can be very useful. In PDF transport methods, the fluid behavior resulting from the interaction between reactive scalars and a turbulent velocity contribution leads to complex management of statistical data. To accommodate this situation the state is defined with interdependent variables including velocity distributions. These variables are not assumed independent leading to a complex joint PDF. Unfortunately, the handling of a complex PDF with multiple
interdependent variables is challenging. As a result the joint PDF with statistically dependent variables tends to only be seen in PDF transport methods.

PDF and FDF transport methods have shown a great deal of promise for many years. The most appealing aspect of these methods is the ability to capture the multivariate PDF which describes a more complex relation between reactive scalars and turbulent velocity components. These applications which transport a single joint PDF, unfortunately, must account for a large dimensionality requiring creative solutions to solving an equation including a large number of interdependent variables. The Lagrangian Monte Carlo method is the most popular solution to this problem; however, as with many of these solutions it is not perfect for all applications. The Lagrangian Monte Carlo method solves the n-dimensional problem by reducing the transport to a three-dimensional problem with the particles representing the fluid and its PDF being updated via a Lagrangian transport equation. The values of the PDF are then conditioned on previous quantities allowing for a closed solution. Albeit simplified, these methods are still quite complex and require a high degree of computational overhead. In most of the studies represented herein, scalar probabilities are assumed statistically independent, which means there is no need for highly dimensional PDFs and complex alternate solutions.

D2. **Histogram distributions**

An alternative to using a mathematical function to describe the distribution of a given scalar is to determine the distribution from datasets generated experimentally or through highly resolved simulations. A simple tool used to represent a distribution from a given dataset is a histogram. A histogram is a discrete mechanism using simple arithmetic to represent a piecewise continuous distribution function based on data provided (Ryan, 2007). The
The functional form of a histogram is expressed as a normalized sum of values for a given coordinate (Faber, 2012).

$$P(x_j) = \frac{1}{n} \sum_{i=1}^{n} 1 \quad x_j \leq X_i < x_{j+1}$$
$$x_j > X_i; X_i \geq x_{j+1}; \quad (9.20)$$

$X_i$ are the samples located in the range from $x_j$ to $x_{j+1}$. From this definition, it is apparent that discontinuities can occur when there are values of $x_j$ without any samples. Discontinuities are not desirable for applications requiring smooth functions, so organizing data using histograms is challenging. The data must be grouped such that there are no discontinuities in the distribution. Even though many turbulent domains contain reasonably sized data clusters in key parts of the flow field, tools using histograms must still be sensitive to gaps in the sample data. Solutions must select the best number of samples in order to build useful distribution. When fewer sample ranges are selected the functional representation is more consistent, but the larger regions can dilute the samples and smear the results. Ideally, a balance must be found that captures the necessary information without too many numerical challenges.

In addition to issues with discontinuities, very large datasets can be costly to manage with complete histograms. Effective reduction techniques can capture a distribution from a sample set rather than forcing the method to maintain a histogram of data. These methods provide a functional definition of the PDF which eliminates discontinuity issues associated with sparse data and reduces the storage overhead for future use. A kernel density function (KDF) is a linear combination of multiple single modal distributions selected based on key aspects of the sample data. Silverman found that a KDF is very good at capturing multi-modal distributions, thus accurately predicting any distribution given a large enough dataset (Silverman, 1981). A method applying a KDF uses the sample data to select accurately which
Appendix E – ODT Modeling: Additional information

E1. LES Filtering

For LES closure it is necessary to provide state vectors which are both spatially resolved variables as well as filtered variables. Filtered variables can be calculated directly from the spatially resolved ODT solution by applying the filter function of choice. At a minimum, a 1D filter provides sufficient information because the more important turbulent statistics are in the transverse direction. However, in some cases downstream information may also be of value. With downstream distance as a function of the time, the equivalent of a 2D LES filter is possible by applying the filtering algorithm over consecutive time slices.

\[
\bar{\Psi} = \iiint G(x_i - \xi, t_n - \eta)\Psi(\xi, \eta)d\xi d\eta
\]  

(9.21)

The only real limitation with this method of filtering is the computational overhead. Collecting statistics and filtering is computationally expensive, so these operations are generally not executed for each time step. Alternatively, the collection is performed in a more granular fashion. The solution is advanced to a certain point in time, and then the collection process is executed. This minimized approach balances collecting enough data and not increasing the solution overhead considerably. When applying the 2D filter from Eq. (9.21), the time slices triggering a data collection event must be as granular as the ODT grid such that \(\Delta tU_{bulk} \approx \Delta x\). Furthermore, enough slices must be stored in order to represent the downstream LES grid size.
The additional collection granularity increases the computational overhead, and storing enough ODT domains to capture the LES width requires additional memory. These issues must be considered when determining if the added information captured by a 2D filter is absolutely necessary or if a 1D filter is sufficient for the target application. This choice may result in information lost within the available time slices, but balancing information gathered with the computational cost is necessary. Fortunately, analysis of homogeneous turbulence assumes that fluctuations are equivalent in all directions. Therefore, a symmetric filter should render the same result regardless of which direction considered. Even though a 1-D filter applied to an ODT solution does not result in the same accuracy as that applied to a DNS solution, the additional information gained from the enhanced solution capabilities of ODT provides a nice balance, when compared to DNS capabilities.

E2. State Vector and Scalar Distribution Selection

When considering which type of distribution function to apply to a turbulent combustion problem, the statistical method should be considered in conjunction with the composite state-space. Scalar and vector quantities within a RANS domain are the result of ensemble averaging over a random set of realizations of the same simulation. These values are considered to be time and space dependent where the instantaneous quantity is represented as the mean plus a fluctuation: \[ u_i = \langle u_i \rangle + u_i' \]. Quantities within an LES domain are the result of an instantaneous spatial filter. Given an ensemble of quantities, a probability density function (PDF) for RANS is the probability that a particular instantaneous value would contribute to a resulting RANS value: \( P(u_i \Rightarrow \langle u_i \rangle) \). Stated differently, RANS variables are
mean quantities dependent on space and time, and the PDF expresses the probability of an instantaneous value existing at that same location and time. The single point distribution does not include frequency and length scale information; however, this limitation is expected within RANS simulations due to the general smearing effects (Pope S. B., 1985).

On the other hand, LES solutions capture instantaneous values which are functions of space and time. There is no averaging in LES; instead, the filtering process removes higher frequency values that were included in the spatially resolved domain leaving only solution values in the LES domain. Finely resolved values are expressed as fluctuations from filtered quantities: \[ u_i = \bar{u_i} + u'_i \]. Similarly to RANS, LES requires use of a density function to predict the fluctuating values within the filtered domain. While the purpose is the same -- to provide the likelihood that at a resolved value would contribute to a resulting filtered value \( F(u_i \rightarrow \bar{u_i}) \) -- the definition may vary based on the purpose and the context. Pope defines the filter density function as filtering a fine grained density providing a distribution function which is a function of the composition array, location and time.

\[
P(\Psi, x, t) = \int_{-\infty}^{\infty} \delta(\psi - \phi(x, t))G(x - x')dx'
\]  
(9.22)

This definition is necessary for methods that intend to transport the distribution function. Transported FDFs are dependent one the spatial domain as well as the composition space, thus the definition must include this information as well.

Tabulated methods do not require any spatial information in the distribution. Instead, the distribution is reduced to a function of state variables and their associated moments. Without a good method to capture such information, researchers have turned mainly to prescribed functions that have a similar form (Cook & Riley, 1994; Pitsch & Steiner, 2000;
Ranganath & Echekki, 2008). For turbulent combustion, the distribution function of choice has been the \( \beta \)-PDF. The \( \beta \)-PDF is a useful function that expresses a distribution in terms of the resolved variable with the first and second moment. The first moment is essentially the filtered version of the variable equivalent to that expressed in LES space. The second moment is the variance of the filtered variable. This term illustrates the range of fluctuations within a filtering operation.

In the present study, data needed to predict turbulent statistics are gathered from a set of ODT realizations defined on a DNS sized 1D grid. The only difference between ODT generated statistics for an FDF and those obtained from DNS and experiments are the dimensions of the filter. Even though the data within ODT represents a 3D flow, the data points are defined in only one dimension. The LES filter within ODT is a 1D filter, while the DNS filter is a volume based filter. The simplest filter that can be applied is a box filter.

\[
\bar{\psi}(x) = \bar{\int_{x-\Delta/2}^{x+\Delta/2} \frac{1}{\Delta} \psi(x') \, dx'}
\]  

(9.23)

This type of filter gives equal weight to all of the contributing values within the LES sub-grid \( \Delta \). More complex filters may change the contributions from unfiltered sources, but the grid size is what determines the reach of the correlated statistics. The data collected in this study is organized in an ensemble to generate distributions of independent variables. These distributions are then either represented in a tabular FDF (generated from histogram methods) or a KDF learned from the given samples. In order to capture the effects of variance, the ensembles are organized based on whether a selected sample contributes to a distribution defined for that variance. The variances categorizing the scalar distributions must be filtered within ODT because variances within LES are also filtered. The challenge with using the
filtered variance is finding a consistent tractable definition that correlates best with the actual data. Within the ODT domain, the variance as defined by Eq. (2.44) is calculated from spatially resolved variables to correlate distributions with a selective variance.

Appendix F – Non-Premixed Flame Background

F1. Non-premixed flame studies

Non-premixed flames have been studied in a variety of experimental configurations for many years. These configurations include tests such as a simple pan fire, the counter flow diffusion flame, the co-flow jet flame, and the piloted non-premixed jet flame (McCaffrey, 1979; Peters, 2000; Barlow R., Frank, Karpetis, & Chen, 2005). With each having a different purpose, selecting the flame configuration which best represents the phenomena of interest is important. When working with ODT, the turbulence-combustion interaction is the focal point of interest, and thus the piloted non-premixed jet flame is most suitable to validate theoretical research. For almost 20 years, data has been accumulated and analyzed through a multitude of studies surrounding the piloted jet diffusion flame (Barlow & Frank, 1998; Barlow & Frank, 2007). As a result of collaborations via the Turbulent Non-premixed Flames international workshops, the Sandia family of flame configurations have been the case study of choice to validate different simulation models (Pitsch & Steiner, 2000; Echekki T., Kerstein, Dreeben, & Chen, 2001; Sheikhi, Drozda, Givi, & F.A. Jaberi, 2005). The Sandia Flame is a piloted non-premixed flames that is operated under a variety of turbulent conditions making it a good choice for studying flame-turbulent interactions. Thanks to the many researchers who have
conducted experiments and organized the data, the Sandia flames provide a nice dataset for validating computational research.

F2. Turbulent Non-premixed Flames (TNF)

Established in 1996, the TNF is an internationally organized effort to maintain consistency in the research performed to study turbulent chemistry interactions within turbulent non-premixed flames (Barlow R., 2016). Many of the first workshops focused on gathering experimental data needed to analyze the phenomena as well as validate computational models. More recently, the focus has shifted to development of closure models for LES and other more complex flame configurations. Following construction of datasets for hydrogen-air flames, additional experiments were performed for methane-air, propane-air and others. There are two main structures that are of importance with the TNF: jet diffusion flames and bluff body flames. The turbulence with jet diffusion flames is the result of the velocity shear produced by a round jet, while the bluff body flow uses a round structure impeding the flow to generate a recirculation zone amidst the fuel flow. While different in construction both provide the same features in that they are controlled environments that facilitate measuring the interactions between turbulence and combustion. Each flame type renders turbulent structures that are good for validating ignition, extinction and re-ignition.

In the late 1990s (Barlow & Frank, 1998) conducted a series of experiments to capture measurements of scalars in the piloted jet diffusion flame at varying levels of turbulence. This apparatus which was designed at the University of Sydney uses a combination of Raman and Rayleigh scattering along with laser-induced fluorescence to measure temperature, flow velocities and species concentrations (Masri, Dibble, & Barlow, 1996). Furthermore, the
piloted jet configuration was the focus of many different modeling studies including studies on PDF transport (Hinx, Hassel, & Janicka, 1998), studies on CMC (Roomina & Bilber, 1998), an introduction to ODT (Echekki & Kerstein, 1998), and studies using steady and unsteady flamelets (Pitsch, Chen, & Peters, 1998). In the ten years following additional research was performed to improve the reduced reactions mechanisms, study the extinction/re-ignition characteristics and the mixing models applied throughout. The bluff body and swirl flames were later added to the mix of configurations used to study the chemistry-turbulence interaction. Finally, in more recent years, the studies have been expanded to include stratified flows as well as opposed jet and piloted DME flames.

Numerous studies have validated model results through simulating Flame D. (Pitsch & Steiner, 2000) validated the lagrangian flamelet model using the non-premix CH$_4$ combustion in the Flame D configuration. In this study, they adapted a spherical DNS code which was created specifically for the axial jet format (Boersma, Brethouwer, & Nieuwstadt, 1998). Further studies expanded this model to better capture finite chemistry effects exhibited with Flame E and F also using the spherical LES code. At the Imperial College in London, an in-house code was designed to perform the stochastic calculations needed for the Eulerian Monte Carlo method (Jones & Prasad, 2010). Formally named BOFFIN-LES, this code is a block structured finite volume code specifically designed to solve the PDF transport equations needed for a Large Eddy Simulation. Similarly, Skeikhi applied a hybrid finite-difference Monte-Carlo solver to the Sandia Flame D to validate a LES-FDF model (Sheikhi, Drozda, Givi, & F.A. Jaberi, 2005). This method combined a simplified finite difference solution with a corresponding Monte-Carlo simulation of the same problem. Finally, in 2005 Navarro-Martinez validated the CMC method by simulating the Sandia Flame D condition using the
BOFFIN code mentioned above. Navarro-Martinez solves the conditionally filtered species transport equations using presumed PDF for each scalar and classic solutions to the sub-grid fluxes.

One common thread throughout each of these studies is the method by which results are evaluated and analyzed. The experimental results from the Barlow and Frank experiments are compared with results extracted from model controlled simulations. Interestingly though many have similar shortcomings some are stronger in areas where others are weak. None are absolutely perfect in predicting of certain turbulent statistics; however, due to the nature of data accumulation, these comparisons are expected to be similar at best. This study analyzes results in comparisons with experimentally gathered data. First the time averaged axial and radial profiles are compared with experiments. Then conditional variables are analyzed through 1D contours.