RANS-SLFM and LES-SLFM numerical simulations of turbulent non-premixed oxy-fuel jet flames using CO2/O2 mixture

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RANS-SLFM and LES-SLFM numerical simulations of turbulent non-premixed oxy-fuel jet flames using CO$_2$/O$_2$ mixture

by

Adel Alghamdi

A thesis submitted to the graduate faculty

in partial fulfillment of the requirements for the degree of

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Major: Chemical Engineering

Program of Study Committee:
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ABSTRACT

The focus of this work was to study the structure of multiple turbulent flame configurations using the steady laminar flamelet model (SLFM) coupled with Reynolds-averaged Navier-Stokes (RANS) and large eddy simulation (LES) transport equations. A detailed chemistry mechanism (GRI 3.0) was used in the formulation of the flamelet library. In addition, a probability density function (PDF) approach was used to generate the flamelet table in terms of its mean quantities $\tilde{\phi}(\tilde{Z}, \tilde{Z}{^2}, \tilde{\chi})$ as a function of the Favre-averaged mixture fraction, mixture fraction variance, and the scalar dissipation rate. A beta PDF was assumed for mixture fraction and a delta function distribution for the scalar dissipation rate. This approach ensured that finite-rate chemistry effects were introduced in the turbulent flow calculations. Radial mean and RMS distributions of temperature, mixture fraction, and species mass fractions were predicted at different axial locations for Sandia D and B-1 flames. The simulation results were validated against experimental data (Barlow & Frank 2007; Sevault et al. 2012). The validation study showed that LES/SFLM has better mean and RMS distributions for the B1 flame compared to RANS-SLFM. This was due to the fact that LES has a better representation of mixing than RANS since it resolves the large turbulent scales, which contain the largest amount of kinetic energy and control the mixing process in turbulent non-premixed combustion. Nonetheless, RANS-SLFM produced an acceptable mean profile for the Sandia D-flame for relatively low computational expense. However, mean radial profiles of minor species were not accurately predicted for either flame using RANS-SLFM, while good agreement was obtained with LES-SFLM
CHAPTER 1. INTRODUCTION AND OVERVIEW

Turbulent combustion can be classified into premixed and non-premixed combustion. The major difference is the fuel for the non-premixed configuration is fed separately from the oxidizer stream into the combustion chamber where chemical reactions take place. The study will only focus on the non-premixed flames.

Turbulent non-premixed combustion is employed in many industrial systems for two main reasons. First, it is relatively easier to design and build burners compared to a premixed configuration where complete mixing is not required. Second, it is much safer to operate at a large-scale, such as gas turbines, furnaces, and boilers. Turbulent combustion by nature has complex physics due to the complexity of turbulent flow and the chemical reactions that occur during the combustion process. Thus, strong coupling of both phenomena is a major challenge in the field of computational fluid dynamics (CFD); therefore, there is an interest in using numerical simulation as a research tool to model non-premixed turbulent flames to help improve the energy efficiency of current combustors or testing new technologies.

There are three main simulation strategies used in CFD. Reynolds-Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS). In RANS and LES, turbulent eddies are not completely resolved, so another model is required to resolve those eddies, while in DNS all turbulent scales are resolved to the Kolmogorov scale $\eta$. LES has been extensively used in recent years to model the behavior of turbulent non-premixed flames; because LES computational expense stands in the middle between RANS and DNS. In addition, resolving the large scale of the turbulent flow tend to control most of the statistical properties that
affect the flame structure and chemistry. Furthermore, the level of accuracy that LES can provide predicting the pollutant concentrations which cannot be captured by RANS formulations. Therefore, this study will focus on RANS and LES models coupled with chemistry model to simulate non-premixed flames while DNS will not be included in this study.

1.1 Goals and Motivation

One of the primary motives to study oxy-fuel combustion is global warming. First, oxy-fuel combustion system uses CO₂ as an inert gas with O₂ to reduce the adiabatic flame temperature and prevents NOₓ formations from going into the atmosphere. Second, non-premixed oxy-fuel jet flames are not widely studied in the academic literature. Therefore, in this work, Steady Laminar Flamelet Model (SLFM) was used to simulate Sandia D and oxy-fuel (B1) flames in RANS and LES context with full reaction mechanism GRI 3.0 to predict both flames structure. Results from RANS/SLFM and LES/SLFM were validated against experimental data published in the academic literature. In addition, this study included the investigation of the effects of scalar dissipation rate and inlet conditions on the structure of B-1 flame. Finally, the proposed models can be used to improve the efficiency of the oxy-fuel combustion mode in general, leading to less production of harmful emissions.

1.2 Organization

This work is organized into five chapters. Chapter 1 explored the introduction to non-premixed combustion, background, and motivation for conducting this research. The other chapters have been organized as follows:

Chapter 2: Literature of modeling turbulent non-premixed combustion using RANS and LES approaches has been reviewed. In addition, the chapter includes detailed description of Sandia piloted CH₄/air and oxy-fuel CH₄/H₂ flames, including the experimental setup and measurements.
Chapter 3: theoretical background, formulations of RANS and LES turbulence modeling have been presented. The coupling of mixture fraction transport equations and the scalar dissipation rate with the turbulence models have been discussed. For RANS approach, $k-\varepsilon$ model has been adopted for this work along with the combustion model. The LES approach has been discussed in details including the filtering operations, along with the closure models used for the sub-grid stress and the scalar fluxes. In addition, SLFM formulations have been explained in details, including the PDF presumed shapes for constructing the flamelet tables, and the process flow diagram of SLFM with RANS and LES.

Chapter 4: RANS simulation details including the computational domain, grids, and turbulence model parameters for Sandia D and B-1 flames. The results of RANS/SLFM have been presented for both flames and validated against experimental data for the piloted partially premixed Sandia D flame and the non-premixed oxy-fuel B-1 flame.

Chapter 5: LES computational domain, grids, and boundary conditions have been presented for simulating Sandia D and B-1 flames. Results from LES/SLFM, have been compared against RANS/SLFM approach and the experimental data for Sandia D and B-1 flames. In addition, the influence of the scalar dissipation rate and the inlet conditions on the flame structure of B-1 flame have been discussed. Finally, the concluding remarks of this research and the proposed future work have been presented.
CHAPTER 2. BACKGROUND AND LITERATURE REVIEW

For turbulent flows, different length scales exist to be either resolved or modeled. In RANS, turbulent flow is modeled as ensemble averaged where all turbulent fluctuation scales are modeled; (3.1)which make it less accurate compared to other approaches but the most affordable computationally. In combustion, the turbulent fluctuation is not statistically homogenous. Therefore, RANS approach faces difficulties predicting important aspects of reactive flows (Pitsch & Steiner 2000) & (Pitsch 2002a). However, The fundamentals of RANS models can still be used for other modeling techniques explored in the literature by (Wegner et al. 2004) (Klimenko & Bilger 1999) (Pope 1985) (Veynante & Vervisch 2002). On the other hand, large eddy simulation was first introduced in the 1990s to account for some of the drawbacks of RANS approach dealing with turbulent reacting flows. In LES turbulent flow field is spatially filtered and not ensemble averaged which resolves the large scale of turbulent fluctuations that directly affect the mixing process occur in combustion. However, the smallest scales has to be still modeled to close the sub-filtered terms. LES has been used in many combustion problems including pollutants emissions predictions in gas turbine (Eggenstrieler & Menon 2004), internal combustion of aircraft (Kim et al. 1999) (Moin 2002), flame flashback, blow-off calculations for premixed configuration (Selle et al. 2004) (Sommerer et al. 2004) (Stone & Menon 2003), and instabilities of turbulent flames (Angelberger et al. 2001). However, developments in the theory of LES is still on-going for reactive and non-reactive flows, and major goals are yet not achieved.

In LES, all the instantaneous turbulent scales smaller than the filter size \( \Delta \) will apply a spatial filtering operation to account for the contribution of the unresolved small scales. Likewise, in RANS, a closure model is required to close the Reynold stress terms. Therefore, many models
have been proposed to close the sub-filtered stress terms in LES reviewed by (Meneveau & Katz 2000). There are two advantages of using LES model instead of RANS in turbulent combustion. First, most of the kinetic energy exist within the large turbulent scale that controls the mixing process, is fully resolved in LES. Second, the dynamic sub-filter procedures used in LES decouple the large turbulence scale dynamics from the filtered size $\Delta$, known as dynamic Sub-Grid Scale (SGS) model by (Germano et al. 1991) (Moin et al. 1991). However, in general, we can confidently say that LES, is better than RANS approach because of the accurate prediction of scalar mixing and dissipation rate for non-premixed turbulent combustion flames. To highlight the importance of scalar dissipation rate, (Pitsch 2002b) showed that accounting for the fluctuations of scalar dissipation using LES formulation gave better predictions of flame structure on the rich side compared to RANS.

2.1 Non-Premixed Turbulent Combustion

Many established CFD models have been developed to represent the behavior of turbulent non-premixed flames such as Probability Density Function (PDF) transported models (Pope 1990), Conditional Moment Closure (CMC) model (Bilger 1993), and Laminar Flamelet models (Peters 1984a). Those combustion models mainly differ from each other by the coupling of the reactive scalars with mixture fraction and dissipation rate. Also, both flamelet and CMC models account for the finite chemical rate interactions with turbulent quantities. The focus of this study is to use the laminar flamelet approach first introduced by (Peters 1984b) coupled with Reynold-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) models for the targeted flames: Sandia D and oxy-fuel B1. Flamelet approach can be classified into Steady/Unsteady Laminar Flamelet Models (SLFM) discussed in section 3.3 and Flamelet Progress Variable model (FPV) by (Pierce&Moin 2003), where FPV model uses reaction progress variable instead of scalar
dissipation rate in SLFM model for the construction of the flamelet library. FPV will not be discussed in details for this study, but the basic concept is similar. It is based on viewing the turbulent non-premixed flame as a set of multiple laminar diffusion flames referred to as flamelets, with the assumption that the chemical time scale is much smaller than turbulent flow time scale. Usually, SLFM is implemented along with LES formulation because of the accuracy that LES can provide, compare to RANS. This approach ensures that finite-rate chemistry effects will be introduced using detailed chemical mechanisms such as GRI 3.0. Also, this method is computationally cheap because it decouples chemistry from flow calculations where the flamelet library is generated as a pre-processing step.

2.2 Sandia/TUD piloted CH4/Air Jet Flame

A set of experiments conducted by Sandia National Laboratories in Livermore is considered as a prototypical example of turbulent non-premixed jet flame as shown in Figure 1. The burner dimensions used were 7.2 mm for fuel jet inlet, 18.2 mm for the pilot, and 300×300 mm co-flow rectangular wind tunnel. Then, detailed measurements were achieved for temperature and mass fractions of main species O2, N2, H2, H2O, CH4, OH, CO2, CO, and NO. Furthermore, two-component velocity measurements using a fiber-optic laser Doppler were conducted at the Technical University of Darmstadt (Schneider et al. 2003) using the same burner. The flames ranked from A-F based on changing fuel flow rate, in which only flames D through F are turbulent. Those experiments data were published in Turbulent Non-premixed Flames (TNF) workshops by (Barlow & Frank 2007) as a benchmark used to validate and improve the accuracy of CFD codes and help understand the structure of turbulent non-premixed flames.
2.3 Oxy-Fuel Jet Flames

Similar to the experiments of flames A-F, Sandia National Laboratories have also conducted oxy-fuel jet flame using CO2-diluted oxidizer by (Sevault et al. 2012). Two series of flames were tested using a mixture of hydrogen and methane as fuel as shown in Table 1. For the first three flames, the hydrogen molar content was varied in the fuel from 37% to 55% keeping the jet constant at $Re_{fuel} = 15,000$. The second set kept the $H_2$ molar fraction at 55% and varied $Re_{fuel}$ from 12,000 to 18,000. The burner dimensions were 5 mm inside diameter surrounded by 96.5 mm of laminar co-flow oxidizer. For both sets of flames, the oxidizer has 32% $O_2$ in molar percentage diluted in 68% $CO_2$ kept at 294 K to maintain the fuel/air conditions, which lower the adiabatic flame temperature dramatically compared to pure $O_2$ conditions (Nemitallah & Habib 2013).

*Figure 1* Piloted non-premixed Sandia methane/air turbulent flames by Barlow et al. [1]
Unlike the A-F flames, this experiment does not have a pilot because of the high content of hydrogen that kept the flame attached as well as the squared-ending jet nozzle design. However, in comparison, the measurements were not as detailed. The data include temperature and main species mass fractions of CO₂, CO, O₂, CH₄, H₂O, and H₂. On the other hand, no velocity measurements were conducted for this experiment setup. The goal of the experiments was to measure the local extinction that occurs near the nozzle at different flame conditions. The measurements showed high local extinction with decreasing H₂ %mol content in fuel and increasing jet fuel Reynold number as illustrated Figure 2. In this work, we started by simulating flame B-1 because it is a fully burning flame and has the lowest local extinctions reported, where SLFM was coupled first with RANS transport equations, and then with LES.

<table>
<thead>
<tr>
<th>Name</th>
<th>H₂ mol%</th>
<th>Jet Speed (m/s)</th>
<th>Re_fuel</th>
<th>Coflow Speed (m/s)</th>
<th>Adiabatic temperature (k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>55</td>
<td>98.2</td>
<td>15000</td>
<td>0.778</td>
<td>2250</td>
</tr>
<tr>
<td>A2</td>
<td>45</td>
<td>84.5</td>
<td>15000</td>
<td>0.755</td>
<td>2243</td>
</tr>
<tr>
<td>A3</td>
<td>37</td>
<td>75.8</td>
<td>15000</td>
<td>0.739</td>
<td>2236</td>
</tr>
<tr>
<td>B1</td>
<td>55</td>
<td>78.6</td>
<td>12000</td>
<td>0.622</td>
<td>2250</td>
</tr>
<tr>
<td>B2</td>
<td>55</td>
<td>98.2</td>
<td>15000</td>
<td>0.778</td>
<td>2250</td>
</tr>
<tr>
<td>B3</td>
<td>55</td>
<td>117.8</td>
<td>18000</td>
<td>0.933</td>
<td>2250</td>
</tr>
</tbody>
</table>
In the literature there have been few studies that involve modeling of oxy-fuel jet flames; however, not many CFD models were developed for the flames A-B. In addition, these flames bring new challenges to the modeling of turbulent combustion because of the high content of CO\textsubscript{2} used in the oxidizer that causes the flame to be more prone to extinction. Also, the substantial difference in density between the fuel and the co-flow in the absence of the pilot made it difficult to simulate. Proposed model by (Garmory & Mastorakos 2015) simulating flames A1-A3 using LES/CMC model to capture extinction with reduced chemical mechanism ARM1. Overall, the model showed a good agreement with the conditionally averaged temperature at the location z/d=5 while not an accurate prediction for O\textsubscript{2} and H\textsubscript{2}O mass fraction profiles at the location z/d=3. Therefore, this might indicate the necessity of using detailed chemistry mechanism offered in SFLM. On the other hand, the model over-predicted extinction at both locations z/d=3, z/d=5, respectively, but successfully captured the physical location of the adiabatic flame temperature. Whereas SFLM basic assumptions and formulation do not account for local extinction or re-ignition phenomena, therefore modeling of local extinction will not be the focus of this study. On
the other hand, FPV model can be proposed to capture some level of extinction occurs in the flame A-B. Some preliminary work has been established using LES/FPV prior to writing this thesis simulating B-1 flame; however, a complete study will be proposed later. The study will include the capture of local extinction of B flames and compared to LES/SLFM results.
CHAPTER 3. THEORY AND GOVERNING EQUATIONS

Modeling of turbulent combustion is based on solving a set of governing equations for momentum and scalars. These equations represent the turbulence and chemistry interactions of reactive flows or combustion. This mission of coupling chemistry and turbulence is quite challenging because of the variation of time and length scales in the combustion process. In this section, we will discuss the theory and formulation of SLFM with RANS and LES models.

3.1 Reynolds–Averaged Navier-Stokes (RANS)

The formulation of Reynolds-Averaged Navier-Stokes (RANS) models is based on ensemble averaging of the dependent variables. RANS solves the governing equations of all eddy scales by taking the overall ensemble average of each instantaneous variable. To introduce the concept of ensemble averaging, decomposition of the instantaneous variable \( f \) into mean and fluctuation components expressed as:

\[
f = \bar{f} + f''
\]  

Where the fluctuation \( f'' = 0 \), this decomposition can result into un-closed correlation terms in the balance equations. Density-weighted averages are introduced to account for the high variation of density in combustion, which is known as Favre-averaging. This averaging will lead to a more compact form of equations with fewer un-closed correlations:

\[
\bar{f} = \frac{\rho \bar{f}}{\bar{\rho}}
\]
After using this formalism, the Favre-averaged balance equations for mass and momentum equations become:

\[ \frac{\partial}{\partial t} (\bar{\rho}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{v}_j) = 0 \]  \hspace{1cm} (3.4)

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{v}_j) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{v}_j \bar{v}_j) = -\frac{\partial}{\partial x_j} (\bar{\rho}) + \frac{\partial}{\partial x_j} (\sigma) - \frac{\partial}{\partial x_j} (\bar{\rho} v^* v^*) + (\bar{\rho} g) \]  \hspace{1cm} (3.5)

Where \( \sigma \) is the shear stress tensor and \( \bar{\rho} v^* v^* \) is the unclosed Reynolds stress tensor, which can be closed by using a turbulence model such as Eddy Viscosity Models (EVM). For this study, \( k-\epsilon \) was used as the RANS turbulence model because it is reasonably accurate and simple. The turbulent stress is modeled as:

\[ \bar{\rho} v^* v^* = -2\mu_i \tilde{\gamma} - \frac{2}{3} (\mu_i \nabla \cdot \tilde{v}) \tilde{\delta} + \frac{2}{3} \bar{\rho} \bar{k} \tilde{\delta} \]  \hspace{1cm} (3.6)

Where \( \tilde{\gamma} \) is the Favre-averaged rate of strain, \( \bar{k} \) is the Favre-averaged turbulent kinetic energy and \( \tilde{\delta} \) is the Kronecker delta. The kinetic energy is the key variable representing the turbulent behavior while the turbulent viscosity \( \mu_i \) can be obtained using dimensional analysis. Both are defined as:

\[ \bar{k} = \frac{1}{2} v^* \cdot v^* \]  \hspace{1cm} (3.7)

\[ \mu_i = C_{\mu} \bar{\rho} \frac{\bar{k}^2}{\bar{\epsilon}} \]  \hspace{1cm} (3.8)

Where \( C_{\mu} \) are the empirical constants equal to 0.09. This leads to the Favre-averaged transport equations of \( \bar{k} \) and \( \bar{\epsilon} \) to complete closing the Reynolds stress term of the momentum equation and compute the turbulent viscosity \( \mu_i \), which can be expressed as:
\[
\frac{\partial}{\partial t} \left( \rho \tilde{k} \right) + \frac{\partial}{\partial x_j} \left( \rho \tilde{v} \tilde{k} \right) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla \tilde{k} \right] + P_k - \left( \rho \tilde{e} \right) \tag{3.9}
\]

\[
\frac{\partial}{\partial t} \left( \rho \tilde{e} \right) + \frac{\partial}{\partial x_j} \left( \rho \tilde{v} \tilde{e} \right) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\tilde{e}}} \right) \frac{\partial}{\partial x_j} \left( \tilde{e} \right) \right] + \left( c_{\varepsilon_1} \frac{\tilde{e}}{k} \right) P_k - \left( c_{\varepsilon_2} \frac{\tilde{e}^2}{k} \right) \tag{3.10}
\]

Where \( \sigma_k \) and \( \sigma_{\tilde{e}} \) are the turbulent Prandtl number for \( \tilde{k} \) and \( \tilde{e} \) with the values 1.0 and 1.3, respectively. \( c_{\varepsilon_1} \) and \( c_{\varepsilon_2} \) are empirical constants that have the default values of 1.44 and 1.92 respectively; \( P_k \) is the production of turbulence kinetic energy due to the mean gradient of velocity.

### 3.1.1 Conserved scalar: Mixture Fraction

In RANS there are two additional Favre-averaged equations of the conserved scalar known as mixture fraction \( \tilde{Z} \) and mixture fraction variance \( Z^{n2} \) that needs to be solved. These two quantities are directly involved in the tabulation of flamelet equations used in SLFM. By definition the mixture fraction \( Z=1 \) for fuel and \( Z=0 \) for oxidizer at the inlet of the jet. The transport of equations of Favre-averaged mixture fraction and variance can be written as:

\[
\frac{\partial}{\partial t} \left( \rho \tilde{Z} \right) + \frac{\partial}{\partial x_j} \left( \rho \tilde{v} \tilde{Z} \right) = \frac{\partial}{\partial x_j} \left( \left( \mu_t + \mu_i \right) \frac{\partial}{\partial x_j} \left( \tilde{Z} \right) \right) \tag{3.11}
\]

\[
\frac{\partial}{\partial t} \left( \rho Z^{n2} \right) + \nabla \cdot \left( \rho \tilde{v} Z^{n2} \right) = \frac{\partial}{\partial x_j} \left[ \left( \mu_t + \mu_i \right) \frac{\partial}{\partial x_j} \left( Z^{n2} \right) \right] + C_\varepsilon \mu_i \left( \nabla \tilde{Z} \right)^2 - \left( \rho \tilde{Z} \right) \tag{3.12}
\]

Where \( \sigma_i \) and \( C_\varepsilon \) are model constants 0.85 and 2.85, respectively. The first term in the RHS of equations (3.10) and (3.11) is the molecular diffusion term; the second term in the mixture fraction variance equation is the production term due to the mean gradient of mixture fraction; the third
term on the RHS of equation (3.11) represent the scalar dissipation rate. The mean scalar dissipation rate $\bar{\chi}$ can be expressed in RANS context as the ratio of the shear rate multiplied by the mixture variance (Janicka & Peters 1982) as:

$$\bar{\chi} = C_\chi \frac{\varepsilon}{k} Z^{*2}$$  \hspace{1cm} (3.13)

Where $1.5 \leq C_\chi \leq 3$ but most of the CFD codes uses 2 for turbulent flows in general. In section 5.5, the effects of scalar dissipation and its constant on the flame structure are presented.

### 3.2 Large Eddy Simulation (LES)

This modeling approach is based on capturing the large scale of turbulence using spatial filtering of the instantaneous fields. So generally in LES, turbulence scales are decomposed into resolved scale, and sub-grid scale resulted from applying those filtering operations. The resolved part is captured by solving a set of filtered equations while the small sub-grid scale is modeled.  

The spatial filter for $\Phi$ in LES for quantity $\Phi$ is defined as:

$$\Phi = \int_D G(x-x')\Phi(x')dx'$$  \hspace{1cm} (3.14)

Where $D$ is integration domain and $x'$ stands for the coordinate vector with a given filter size $\Delta$ defined as:

$$G(x-x') = \begin{cases} 1, & \text{if } |x-x'| \leq \frac{\Delta}{2} \\ 0, & \text{otherwise} \end{cases}$$  \hspace{1cm} (3.15)

Nevertheless, a Favre-filtered operator defined as $\Phi = \overline{\rho \Phi}$ applied to the Navier-Stokes equations where unclosed sub-filtered terms will appear. The Favre-filtered mass and momentum balance equations become:
\[
\frac{\partial}{\partial t}(\bar{\rho}) + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{u}_j) = 0
\] (3.16)

\[
\frac{\partial}{\partial t} (\bar{\rho}\bar{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{u}_i \bar{u}_j) = -\frac{\partial}{\partial x_j}(\bar{\rho}) + \frac{\partial}{\partial x_j}(\sigma_{ij}) + \frac{\partial}{\partial x_j}(\tau_{ij}^{SGS})
\] (3.17)

Where:

\[
\sigma_{ij} = 2\bar{\rho}\nu \left[ \bar{S}_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial}{\partial x_k} (\bar{u}_k) \right], \bar{S}_{ij} = \frac{1}{2} \left[ \frac{\partial}{\partial x_j} (\bar{u}_i) + \frac{\partial}{\partial x_i} (\bar{u}_j) \right]
\] (3.18)

Where \( \bar{S}_{ij} \) is the resolved strain rate tensor and \( \tau_{ij}^{SGS} \) can be modeled as:

\[
\tau_{ij}^{SGS} = \bar{\rho}\bar{u}_i \bar{u}_j - \bar{\rho}u_i u_j
\] (3.19)

In the same manner, the filtered mixture fraction \( \tilde{Z} \) can be written as:

\[
\frac{\partial}{\partial t} (\bar{\rho}\tilde{Z}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j \tilde{Z}) = \frac{\partial}{\partial x_j}(\bar{\rho}D \frac{\partial}{\partial x_j} (\tilde{Z})) + \frac{\partial}{\partial x_j}(M^{SGS})
\] (3.20)

Where \( \tilde{D} \) is the eddy diffusivity and the sub-filter \( M^{SGS} \) can be expressed similarly to \( \tau_{ij}^{SGS} \) as:

\[
M^{SGS} = \bar{\rho}\bar{u}_i Z_j - \bar{\rho}\bar{u}_i \tilde{Z}
\] (3.21)

Unlike RANS model, Favre mixture fraction variance \( Z'^2 \) transport equation is not solved, and local equilibrium is assumed to neglect all transport occurs in the physical space (Girimaji & Zhou 1994). Therefore, a simple algebraic model for Favre variance \( Z'^2 \) is written as:
\[ Z''^2 = C_v \Delta^2 (\nabla \hat{Z})^2 \]  

(3.22)

Where \( C_v \) is a constant that can be dynamically computed as proposed by (Moin et al. 1991). However, in this study, we use the value \( C_v = 0.1 \) as recommended for jet flows. Although this variance model, in general, has some issues with other flow types because of the non-validly of the local equilibrium assumption discussed by (Jiménez et al. 2001) (Wang & Tong 2002) (Mellado et al. 2003). Similarly, the filtered scalar dissipation rate usually computed using the same equilibrium hypothesis and modeled as:

\[ \chi = C_\chi D |\nabla Z|^2 \]  

(3.23)

Where \( C_\chi \) is model constant equal 2.0 in LES approach.

### 3.2.1 Closure Model

Several closure models have been proposed to close the sub-grid flux scales terms \( \tau_{ij}^{SGS} \) and \( M^{SGS} \) in momentum and mixture fraction equations, (3.16) and (3.19) respectively. However, the gradient diffusion based model is a widely used to close those terms by (Smagorinsky 1963). The proposed sub-grid scale model for \( \tau_{ij}^{SGS} \) can be expressed as:

\[ \tau_{ij}^{SGS} = 2\mu_i S_{ij} \]  

(3.24)

Where \( \mu_i \), the eddy viscosity, calculated using the help of Smagorinsky model written as:

\[ \mu_i = C_s \overline{\rho} \Lambda^2 \hat{S} \]  

(3.25)

Where \( \hat{S} \) is the magnitude of the rate of strain tensor and \( C_s \) is a constant computed using the dynamic procedure by (Germano et al. 1991)(Moin et al. 1991) with homogeneity assumption in
the azimuthal direction. This involves new definition to \( \tau_{ij}^{SGS} \) using a new filter to the LES filed for the dynamic technique in computing \( C_s \). Where the new sub-grid scale \( T_{ij} \) is modeled as:

\[
T_{ij} = \rho \tilde{\tilde{u}}_i \tilde{u}_j - \bar{\rho} \bar{u}_i \bar{u}_j
\]  

(3.26)

Moreover, the new resolved turbulent stress \( L_{ij} \) known as Leonard stress is written as:

\[
L_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{\tilde{u}}_i \tilde{\tilde{u}}_j
\]  

(3.27)

As results, the dynamic sub-grid scale model \( \tau_{ij}^{SGS} \) becomes:

\[
\tau_{ij}^{SGS} = T_{ij} - L_{ij}
\]  

(3.28)

The constant \( C_s \) then can be computed using the relation proposed by (Lilly 1992) where the constant is independent of the filter width. As results, an equation for the model constant \( C_s \) can be expressed using the tensor relationship as:

\[
C_s = \frac{L_{ij}}{M_{ij}}
\]  

(3.29)

Where \( M_{ij} \) is the model term computed in each computational node and expressed as:

\[
M_{ij} = 2 \bar{\rho} \Delta^2 \left| \mathbf{S}_i \right| \mathbf{S}_j - 2 \bar{\rho} \Delta^2 \left| \tilde{\tilde{S}}_i \right| \tilde{\tilde{S}}_j
\]  

(3.30)

The evaluation of the constant \( C_s \) dynamically can take unphysical negative values. Therefore, the constant is clipped above zero. Also, \( C_s \) is averaged into the direction of homogeneity, in our case, it is in the azimuthal direction. However, the equation (3.27) will be solved using least square and can be written as:
$$C_s = \frac{\langle L_j M_j \rangle}{\langle M_j M_j \rangle}$$  \hfill (3.31)

On the other hand, the mixture fraction sub-grid scale $M_{SGS}$ term is also modeled using the gradient diffusion based hypothesis. The sub-filter is then modeled as:

$$M_{SGS} = D_i \frac{\partial}{\partial x_j} (Z)$$  \hfill (3.32)

Where $D_i$ is the turbulent eddy diffusivity determined from $D_i = \frac{\mu_i}{Sc_i}$ where $Sc_i$ is the turbulent Schmidt number constant set at $Sc_i = 0.7$. However, there are proposed dynamic models for computing the eddy diffusivity $D_i$ using the similar form for computing $\mu_i$. The dynamic procedure for computing the model constant can be calculated as:

$$D_i = C_z \rho \Delta^2 \hat{S}$$  \hfill (3.33)

Where the ratio between $C_z/C_s$ gives the turbulent Schmidt number. Using the same technique computing, the constant $C_z$ dynamically in equation 3.29, the constant $C_z$ can be modeled as:

$$C_z = \frac{\langle L_j M_j \rangle}{\langle M_j M_j \rangle}$$  \hfill (3.34)

Where,

$$L_j = \hat{u}_j \hat{Z} - \tilde{u}_j \tilde{Z}, \text{ and } M_j = 2 \tilde{\rho} \Delta^2 |S| \frac{\partial}{\partial x_j} Z - 2 \tilde{\rho} \Delta^2 \hat{S} \left( \frac{\partial}{\partial x_j} \hat{Z} \right)$$  \hfill (3.35)
3.3 Steady Laminar Flamelet Model (SLFM)

The simple explanation of SLFM is, it represents the non-equilibrium version of Burke-Schuman solution. Both approaches essentially link all reactive scalars to the mixture fraction \( Z \). However, the major difference is that SFLM ignores the chemical equilibrium assumption, and solve for a set of one-dimensional steady diffusion equations as a function of mixture fraction \((Z)\) and scalar dissipation rate \((\chi)\) (Peters 1984a).

There are many advantages of using the flamelet approach. First, calculations of thermochemistry are decoupled from turbulence calculations, since flamelet equations are solved and then stored in a look-up table known as flamelet library. Second, the fact that the finite-rate chemistry effects are included using detailed chemistry mechanism such as GRI3.0, which differentiates this method from other turbulent combustion models. Finally, the model has a low computational expense compared to other combustion models because flamelet equations are solved in one-dimensional space, where it can be used for complex geometry such as turbines or furnaces. On the other hand, SLFM fails in capturing flames behaviors like extinction (where the mixing rate is faster the reaction rate) and flame re-ignition (where mixing rate is slower than reaction rate). However, SFLM model can still produce fairly accurate results predicting the flame structure and emission mass fractions profiles (Pitsch 2006) (Müller et al. 2013).

Figure 3 Configuration of counter-flow diffusion flame
The basic concept of flamelet is that the turbulent flame can be viewed as a multiple ensemble laminar one-dimensional flamelets, where the flame reaction zone is assumed to be smaller than the Kolmogorov length scale $\eta$. The flamelets are generated using the counter-flow configuration shown in Figure 3 and constant diffusion with Lewis number equal to unity. The assumption of ($L_e=1$) is valid in turbulent flames because differential diffusion controls only a thin layer around the reaction zone near the nozzle, as discussed by (Pitsch 2000). On the other hand, the mean quantities of reactive scalars are computed using the pre-assumed joint-PDF of mixture fraction and scalar dissipation rate.

### 3.3.1 Flamelets Governing Equations

The basic derivation of the flamelet equations is based on two strategies. First, co-ordinate transformation of physical space to mixture fraction space shown in Figure 4(a). The transformation is applied to the instantaneous transport equations of temperature and species mass fraction, as $(x_1, x_2, x_3, \tau)$ transforms to $(Z, Z_2, Z_3, \tau)$. The $x_i$ coordinate defined as a normal coordinate to the flame surface and replaced by $Z$, where $x_2$ and $x_3$ are the tangential coordinates and replaced by $Z_2$ and $Z_3$, respectively.

![Figure 4](image)

*Figure 4* (a) co-ordinate transformation of mixture fraction (b) surface of stoichiometric mixture fraction in turbulent jet flame (Peters 1984a)
Second, was reducing the dimensions of the problem by considering only the flame surface normal and neglecting the tangential directions. This was based on the assumption that most of chemistry and temperature change occur near the stoichiometric condition in the normal direction. Therefore, the distribution of mixture fraction in space and time can be represented by the stoichiometric condition, \( Z(x,t) = Z_{st} \) as illustrated in Figure 4 (b).

The governing equations for steady flamelet of temperature \( T \) and species mass fraction \( Y_i \) as function of mixture fraction and scalar dissipation, derived by (Peters 1984a), can be expressed as:

\[
\frac{1}{2} \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} + \omega_i = 0
\]

\[
\frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial Z^2} - \frac{1}{c_p} \sum_{i=1}^{a} h_i \omega_i + \frac{1}{2 c_p} \rho \chi \left( \frac{\partial c_p}{\partial Z} + \sum_{i=1}^{a} c_p \frac{\partial Y_i}{\partial Z} \right) \frac{\partial T}{\partial Z} = 0
\]

Where \( \omega_i \) is the reaction rate provided by the GRI 3.0 mechanism that includes 325 reactions and 53 species, \( h_i \) and \( c_p \) are the enthalpy and specific heat capacity for each species, \( \chi \) is the instantaneous scalar dissipation rate defined as:

\[
\chi = 2 \cdot D |\nabla Z|^2
\]

The scalar dissipation \( \chi \) plays an important role in flamelet modeling where it has the unit \( (1/\text{s}) \), which is also known as the inverse of the characteristic diffusion time scale. Scalar dissipation rate variable has a strong relationship with the mixture fraction and time, which represent the characteristic strain rate of the flame in general. Therefore, it can be defined as
\( \chi = \chi(Z, t) \). An improved version of modeling \( \chi \) include the effect of density fluctuations through the flame, where the conditional scalar dissipation rate can be modeled as (Kim & Williams 1997):

\[
\chi(z) = \frac{a_s}{4\pi} \frac{3\left(\sqrt{\rho_\infty / \rho + 1}\right)^2}{2\sqrt{\rho_\infty / \rho + 1}} \exp\left(-2\left[\text{erfc}^{-1}(2Z)\right]^2\right)
\]

(3.39)

Where \( \rho_\infty \) the density of the oxidizer co-flow is, \( \text{erfc}^{-1} \) is the inverse complementary error function and \( a_s \) the strain rate of counter-flow configuration related to the stoichiometric scalar dissipation related to \( \chi_{st} \) at \( (Z = Z_{st}) \) which can be expressed as:

\[
a_s = \frac{\chi_{st}\pi}{\exp\left(-2\left[\text{erfc}^{-1}(2Z_{st})\right]^2\right)}
\]

(3.40)

Where physically, when the flame is strained, flame thickness decrease and mixture fraction gradient increase in the direction of \( (Z = Z_{st}) \); therefore \( \chi_{st} \) is used as a primary parameter to represent the non-equilibrium behavior. For instance, the \( \lim_{\chi_{st} \to 0} = 0 \) represents the equilibrium chemistry and as \( \chi_{st} \) increase the non-equilibrium behavior increase that causes the flame to extinguish due to the aerodynamic straining. However, a relationship between the Favre-average conditional scalar dissipation \( \tilde{\chi}_{st} \) to the un-conditional \( \tilde{\chi} \) can be expressed as:

\[
\tilde{\chi}_{st} = \frac{\hat{\chi} f(Z_{st})}{\int_0^1 f(Z)p(Z)dz}
\]

(3.41)

Moreover, \( f(Z) \) is the exponential term in equation (3.37) defined as:
\[ f(Z) = \exp\left(-2[\text{erf}^{-1}(2Z)]^2\right) \]  

(3.42)

### 3.3.2 Presumed Shape PDF

This approach is used to compute the mean quantities of scalars \( \tilde{\phi} \) such as (Temperature, species mass fraction, and density) as a function of mixture fraction \( \tilde{Z} \). The integration of the flamelets scalars can be defined as:

\[
\tilde{\phi} = \iint \phi(Z, \chi_{st}) P(Z, \chi_{st}) \, dZ \, \chi_{st}
\]  

(3.43)

Where Favre-average of species mass fraction and temperature can be evaluated as:

\[
\tilde{Y}_i = \iint Y_i(Z, \chi_{st}) P(Z, \chi_{st}) \, dZ \, \chi_{st}
\]  

(3.44)

\[
\tilde{T} = \iint Y(Z, \chi_{st}) P(Z, \chi_{st}) \, dZ \, \chi_{st}
\]  

(3.45)

Where \( \chi_{st} \) is the stoichiometric scalar dissipation rate and the joint PDF of \( P(Z, \chi_{st}) \), both defined as:

\[ P(Z, \chi_{st}) = p(Z) P(\chi_{st}) \]  

(3.46)

The marginal PDF \( P(\chi_{st}) \) is modeled with a Dirac function defined as \( P(\chi_{st}) = \delta(\chi_{st} - \tilde{\chi}_{st}) \), where a log-normal distribution considered to be more physical and can be described as:

\[ P(\chi_{st}) = \frac{1}{\chi_{st} \sigma \sqrt{2\pi}} \exp\left(-\frac{\ln \chi_{st} - \mu}{2\sigma}\right) \]  

(3.47)
Where \( \mu \) is parameter related to the Favre-average, defined as

\[
\tilde{\chi}_{st} = \int_{0}^{\infty} \chi_{st} P(\chi_{st}) d\chi_{st} = \text{Exp}\left(\mu + \frac{\sigma^2}{2}\right)
\]

Moreover, the marginal PDF shape for mixture fraction can be described as \( \beta \)-PDF distribution given by:

\[
P(Z) = Z^{\alpha-1}(1-Z)^{\beta-1} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) \Gamma(\beta)}
\]

Where \( \beta, \alpha \) are the \( \beta \)-PDF parameters and \( \Gamma \) is the gamma-function written in terms of mean mixture fraction and its variance:

\[
\alpha = \bar{Z}\gamma
\]

\[
\beta = (1 - \bar{Z})\gamma
\]

where

\[
\gamma = \left(\frac{\bar{Z}(1 - \bar{Z})}{\bar{Z}^2} - 1\right) \geq 0
\]

There are different combinations of plotting the beta pdf function based on the parameters \( \bar{Z} \) and \( \gamma \) are shown in Figure 5. It can be seen that for a small value of \( \bar{Z}^2 \) (large \( \gamma \)), it approach the Gaussian distribution. On the other hand, it develops a singularly solution at the boundary \( Z = 0 \) when \( \alpha < 1 \) and at \( Z = 1 \) when \( \beta < 1 \).
3.3.3 Generation of flamelet library

The flamelet library generation is in four steps as illustrated in Figure 6. The first step applies the coordinate transformation to the instantaneous scalar transport equations in physical space to mixture fraction space. Then, a construction of look-up table of instantaneous quantities $\phi(Z, \chi)$ as function mixture fraction and scalar dissipation rate. The step before the last uses the pdf statistical approach to generate the flamelet library in terms of the mean quantities of scalars $\phi(\bar{Z}, \bar{Z}^2, \bar{\chi})$ as function of Favre-average mixture fraction, variance, and scalar dissipation rate. Finally, the mean flamelet library $\bar{\phi}(\bar{Z}, \bar{Z}^2, \bar{\chi})$ is linked directly to the turbulent flow calculations at each grid point using the equations (3.10, 3.11, and 3.12) for RANS approach and the equations

---

**Figure 5** shapes of beta-function Pdf for different parameters $\tilde{Z}$ and $\gamma$ (Peters 1984a)
(3.19, 3.21 and 3.36) for LES approach. However, the main assumptions used in the construction of flamelet library were:

- Neglect the tangential directions of mixture fraction transformation.
- Neglect the fluctuations of the scalar dissipation rate $\chi''^2$ of the delta pdf function.
- Use stoichiometric scalar dissipation $\chi_{st}$ as the base parameter since most of the chemistry occur around stoichiometric condition.

**Figure 6** Modelling flowchart using SLFM with RANS and LES context
CHAPTER 4. RANS SIMULATION DETAILS

RANS simulations of Sandia D and B-1 flames were performed along with SLFM, then compared against published experimental data by (Barlow & Frank 2007 & Sevault et al. 2012). The Sandia D-flame configured as a partially premixed flame where the air is mixed with the fuel stream to prevent soot formation and help with the flame stability. Oxy-fuel B1 flame, on the other hand, is a non-preamixed flame using H2/CH4 fuel mixture. More details about the computational domain, mesh and inlet conditions are discussed below in more details.

4.1 Sandia D-Flame Simulation Setup

Sandia D flame has Re=22400 with a jet velocity of 49.6 m/s surrounded by a pilot and a laminar co-flow stream with the velocities of 11.4 and 0.9 m/s, respectively. The flame geometry and dimensions are shown in Figure 7. A 2-D axisymmetric plane was considered for the computational domain with 180,000 structured cells, and local refinement at the inlet that grows radially, where the smallest cell size was 0.3 mm and the largest was 5 mm. Also, mesh sensitivity analysis was performed to compute an independent steady state solution.
Simulation and experimental measurements used for the boundary conditions are listed in Table 2. The simulation results were compared with the Favre-averaged scalar measurements of the radial profile at the locations x/d=1, 15, 30, 45, and 60. ANSYS Fluent version 16 was used as the incompressible solver with the realizable $k-\varepsilon$ turbulence model. The realizable turbulence model was used to accurately predict the jet spreading rate as suggested by (Shih et al. 1995). All of the turbulence model constants were set to the default values except for $c_{\varepsilon_2}$=1.9 was changed to $c_{\varepsilon_2}$ =1.8 as suggested by (Pfeiler & Raupenstrauch 2010). All seven RANS equations had convergence criteria of $10^{-5}$ normalized residual.

On the other hand, SLFM model was used as the combustion model where the pre-calculated flamelet table was linked to RANS transport equations at every grid point. The GRI3.0 chemical mechanism was coupled during the solving of the flamelet equations to provide the reaction rate required by 52 species and 325 reactions. The scalar dissipation range from near equilibrium value to the extinction limit of 530 (1/s). The flamelet library was constructed using 200 points of mean
mixture fraction and mixture fraction variance. A beta function was used to describe the PDF distribution of mixture fraction, and delta function for the scalar dissipation PDF. The flamelet library contained Favre-averaged mixture fraction, temperature, species mass fraction and density. The table also contained molecular diffusivity and viscosity computed and stored from the mixture properties. All tabulated values of scalars were called in each grid point based on the mean mixture fraction, mixture fraction variance and scalar dissipation rate from the flow calculation.

Table 2 Boundary conditions based on measurements for Sandia D (Barlow & Frank 2007)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel jet diameter [mm]</td>
<td>7.2</td>
</tr>
<tr>
<td>Pilot diameter [mm]</td>
<td>18.2</td>
</tr>
<tr>
<td>Fuel composition CH₄/air [vol.%]</td>
<td>25/75</td>
</tr>
<tr>
<td>Pilot mixture fraction</td>
<td>0.27</td>
</tr>
<tr>
<td>Fuel mean jet velocity [m/s]</td>
<td>49.6</td>
</tr>
<tr>
<td>Coflow mean velocity [m/s]</td>
<td>11.4</td>
</tr>
<tr>
<td>Pilot mean velocity [m/s]</td>
<td>0.9</td>
</tr>
<tr>
<td>Fuel Temperature[K]</td>
<td>294</td>
</tr>
<tr>
<td>Oxidizer Temperature [K]</td>
<td>291</td>
</tr>
</tbody>
</table>

4.2 Oxy-fuel B-1 Flame Simulation Setup

The oxy-fuel B-1 flame has a lower Reynolds number than Sandia D of (Re=12000) with fuel jet velocity of 78.6 m/s and 0.622 m/s for the co-flow stream. Unlike flame D, the B1 flame does not include a pilot stream, because of the large quantity of hydrogen used that kept the flame attached. A 2-D axisymmetric plane was used for B-1 flame with the dimensions shown in Figure 8. The fuel jet diameter was 5 mm surrounded by 96.5 mm co-flow placed at the top of a squared wind tunnel with 20 ×20 ambient air flow. The wind tunnel inlet was treated as a wall boundary since the experiment setup ensured that no early mixing with ambient air occurs lower
than the location $x/d=20$. A structured mesh was generated for the flame B-1 configuration with 160,000 grid points were the smallest cell size was 0.25 mm and the largest was 10 mm, and grow radially from the jet inlet.

![Diagram](image)

**Figure 8** Oxy-fuel B-1 Flame Geometry, all dimensions are in mm.

The simulation conditions are listed in Table 3 and results were compared with all reported experimental measurements at the locations $x/d=1, 3, 5, 10,$ and 20. Similar to RANS setup for Sandia D, the realizable $k-\varepsilon$ turbulence model was used with the standard constants, and no modifications have been made except for the turbulent Schmidt number $\sigma_t$, changed from the standard value of 0.85 to 1.6. The value for $\sigma_t$ can vary based on the type of flow and geometry in RANS calculations according to (Tominaga & Stathopoulos 2007). Modifying the mixing constant, improved the prediction of flame thickness and the physical location of the adiabatic flame temperature. On the other hand, the SLFM was used for B1 flame with the same
configuration used for flame D. The extinction scalar dissipation rate for B1 was 61 (1/s) since the B1 flame is a much weaker flame compared to Sandia D-flame. In addition, the absence of the pilot stream and using CO2 made this flame more prone to extinction. However, other flames like B3 and A3 have more extinction as shown in Figure 3. Finally, all seven RANS equations had convergence criteria of $10^{-5}$ normalized residual.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel jet diameter [mm]</td>
<td>5</td>
</tr>
<tr>
<td>Co-flow diameter [mm]</td>
<td>96.5</td>
</tr>
<tr>
<td>Fuel composition H2/CH4 [Mol.%]</td>
<td>55/45</td>
</tr>
<tr>
<td>Fuel jet mean velocity [m/s]</td>
<td>78.5</td>
</tr>
<tr>
<td>Co-flow mean velocity [m/s]</td>
<td>0.622</td>
</tr>
<tr>
<td>Fuel Temperature[K]</td>
<td>294</td>
</tr>
<tr>
<td>Oxidizer Temperature [K]</td>
<td>294</td>
</tr>
</tbody>
</table>

**4.3 RANS Results**

The laminar steady flamelet model SLFM was applied with realizable $\tilde{k}$-$\tilde{\varepsilon}$ in a 2D axisymmetric plane to predict the mean distribution of temperature, mixture fraction, and species mass fraction for the Sandia D and B-1 flames. Simulation results were compared with experiment data at different axial locations and the main species investigated were CO$_2$, O$_2$, CH$_4$, NO, CO, H$_2$O, and H$_2$. 
4.3.1.1 Sandia D-Flame Results

Realizable $\tilde{k} - \tilde{\varepsilon}$ model coupled with SLFM was able to reasonably predict the mean radial temperature at different axial locations as shown in Figures 9. However, the calculations using the standard turbulence model constants tend to over-predict kinetic energy according to Pfeiler et al. (Pfeiler & Raupenstrauch 2010), which was not included in this study, but the results using $c_{\varepsilon_2} = 1.8$ were reproduced. The over-prediction of temperature at location x/d=30 in the centerline was due to the inaccuracy of predicting the mixing of fuel and air at that location as illustrated in Figure 10, though it was reasonable relative to the computational expense. On the other hand, the over-prediction of temperature could also be due to the low scalar dissipation at the location x/d=30. Similar behavior was also seen for x/d=45. This indicates that the flow calculation of mixture fraction, mixture fraction variance, and scalar dissipation can dramatically influence the temperature and species mass fraction profiles. Therefore, an accurate representation of mixing is usually required for turbulent non-premixed flames since it is dominantly controlled by mixing process. LES is usually used for modeling turbulent non-premixed flames. However, RANS can still provide fair results compare to the time required to run those calculations.
Figure 9 Radial mean profile for temperature at x/d=1 (top left), x/d= 15 (top right), x/d=30 (bottom left) and x/d=45 (bottom right): red points are experiment data of Sandia D from (Barlow & Frank 2007), solid line is simulation results from RANS/SLFM.
Figure 11 shows that the over-prediction of temperature at location $x/d=30$ led to more consumption of fuel and oxidizer mass fractions. In addition, the mean radial emission profiles of NO and CO were not predicted accurately due to the invalidity of the turbulence model; more plots and flame contours are posted in Appendix A. Consequently, improving the accuracy of the turbulent flow calculations lead to capture the flame structure more efficiently, for instance, using LES/SLFM instead of RANS/SLFM discussed in chapter 5. LES offers different mixing representation that resolves the large scale of the turbulent flow and not solve for mixture fraction variance transport equation; rather it is modeled by equation (3.21).
Figure 11 Radial distribution of CH4 mass fraction (top left), O2 mass fraction (top right), NO mass fraction (bottom left), and CO mass fraction (bottom right) at location x/d=30: red points are experiment data from (Barlow & Frank 2007), solid line is simulation results from RANS/SLFM.
4.3.1.2 Oxy-fuel B-1 Results

The steady flamelet model was also applied with the realizable \( \tilde{k} - \tilde{\varepsilon} \) model to simulate the B-1 flame with the standard value of Schmidt number 0.85 and the modified value of 1.6. The radial temperature profile was under-predicted at all locations except for \( x/d = 20 \) as shown in Figures 12. The same argument mentioned earlier can be made for a B1 flame using RANS/SLFM, where mixing and scalar dissipation rate was not accurately predicted as illustrated in Figure 13. However, the temperature profile was mainly affected by the high prediction of scalar dissipation rate \( \tilde{\gamma} \) which exceeds the extinction limit of 61 (1/s) as shown in figure 14. The flame sensitivity to the scalar dissipation rate will be discussed in more details in section 5.4, where the RANS solution was validated against different values of constant \( C_\gamma \) in equation (3.13). However, studying the effect of scalar dissipation using the RANS model was not the focus of this study. Although, the predictions of B1 flame has improved by lowering the scalar dissipation rate computation using the RANS/SLFM approach as discussed in section 5.4. On the other hand, more flexibly was offered in the LES model; OpenFoam was used along with SLFM, and the tabulation of chemistry was by FlameMaster code. In LES, the scalar dissipation was modeled as:

\[
\tilde{\gamma} = C_\gamma D_z \nabla Z \cdot \nabla Z,
\]

resulted in a better mean profile of temperature and species mass fraction discussed in chapter 5. Overall, the RANS results improved in the downstream of the flame, specifically at the location \( x/d = 20 \) since the effect of \( \tilde{\gamma} \) start to diminish at the location.
Figure 12 Radial mean profile for temperature at $x/d=3$ (top left), $x/d=5$ (top right), $x/d=10$ (bottom left) and $x/d=20$ (bottom right): red points are experiment data of B-1 from (Sevault et al. 2012), solid line simulation results (Black =1.6, Green =0.85).
Figure 13 Radial distribution of mixture fraction (left) and mixture fraction variance (right) at location x/d=3: red points are experiment data of B-1 flame from (Sevault et al. 2012), solid line simulation results (Black =1.6, Green =0.85).

Figure 14 Radial distribution of scalar dissipation at axial location x/d=5 (left) and x/d=10 (right): solid line simulation results (Black =1.6, Green =0.85).
On the other hand, the radial distribution of species mass fraction was not accurately predicted because of the under-prediction in temperature. Figure 15 shows more consumption of CH₄ and O₂ mass fraction at the location x/d=10, due to the higher temperature predicted when using the standard value of turbulent Schmidt number equal to 0.85 and decreased with $\sigma_t = 1.6$ as illustrated in Figure 12. However, the standard value of $\sigma_t$ seems to have better agreement with the radial distribution of species mass fraction at the location x/d=10, while the same behavior of temperature profile downstream was seen for the mean profile of species mass fraction with the $\sigma_t = 1.6$ at the location x/d=20. This indicates that mixing and scalar dissipation effects on the flame structure downstream are minor, since the flame becomes more homogenous, starting from the location x/d=20. Unfortunately, there are no experimental measurements after x/d=20 to confirm this conclusion. However, by comparing with flame D at location x/d=60 in Appendix A where the fuel was mostly consumed at that location. The mean profile for temperature and major species mass fraction were relatively reasonable except for the species NO and CO radial profiles which are hard to capture using RANS formulation. Therefore, the similar profile for B1 flame is expected in the downstream, specifically after x/d=20, which suggest that the flame structure downstream is mostly controlled by chemistry and not by the turbulent flow calculations. More plots of B1-flames using RANS/SLFM at x/d=1 are posted in Appendix B including contour plots.
Figure 15 Radial distribution of CH4 mass fraction (top left) and O2 mass fraction (top right) at location x/d=10, CH4 mass fraction (bottom left) and O2 mass fraction (bottom right) at location x/d=20. red points are experiment data of B-1 flame from (Sevault et al. 2012), solid line simulation results (Black =1.6, Green =0.85).
4.4 Conclusion

RANS/SLFM was used for Sandia D and B1 flames and compared against experimental results by (Barlow & Frank 2007) and (Sevault et al. 2012) respectively. Sandia D simulation results showed acceptable agreement at multiple axial locations of temperature and major species mass fractions, while not accurate prediction of the radial mean distribution of NO and CO species. On the other hand, B1 flame showed reasonable radial profile at the location x/d=20 where the Schmidt number was set to 1.6, while under-predicted temperature near the nozzle which influenced the species radial distribution as well. Both flame structure were affected by the prediction of scalar dissipation rate and mixing parameters. However, downstream of both flames seems to be affected more by chemistry and not by the flow calculations. In next chapter, different representation of mixing is proposed using LES/SLFM, where the mixture fraction variance transport equation is not solved, and the scalar dissipation rate is computed from the equation (3.23) as opposed to the equation (3.13) for RANS. Next chapter also includes the study of variant inlet velocity condition and its effects on the flame structure.
CHAPTER 5. LES SIMULATION DETAILS

In this chapter, LES has been used along with SLFM to simulate B1 flame, while not performed for the Sandia D flame since it has been extensively studied in the past years. However, we will explore the recent research that involves simulating Sandia D using LES/SLFM and compared against RANS/SLFM predictions. In additions, the chapter includes the influence of scalar dissipation rate and inlet velocity condition on the flame structure. UmFlameletFoam by (Malik Hassanaly et al.) has been used for the LES calculations along with FlameMaster for construction the flamelet library. On the other hand, computational domain, grids and boundary conditions used by LES/SLFM to simulate B1 flame are discussed.

5.1 LES/SLFM for Sandia D Flame

As part of numerical simulation development of modeling turbulent combustion, Sandia D has been the benchmark for most of the validation studies of the CFD codes. Large eddy simulation was performed for the piloted methane/air flame (sandia D) coupled with SLFM by (Clayton & Jones 2008). The simulation results showed minor differences compare to RANS model in the prediction of the radial mean profiles of temperature, mixture fraction, and major species. However, better prediction of CO and NO radial profiles were captured accurately using the LES formulation with GRI 2.11 as illustrated in Figure 16. In addition, the study includes the comparison between the dynamic and standard Smagorinsky models. The results suggested that the standard Smagorinsky model over-predicted of the velocity fluctuations near the nozzle, while an accurate profile of velocity fluctuations achieved using the dynamic closure (Clayton & Jones 2008). Therefore, the dynamic procedure for computing the constant $C_s$ in equation (3.29) will also be used for simulating B1 flame to calculate the turbulent eddy viscosity of equation (3.23).
5.2 Simulation Setup for B-1 Flame

Different representations of mixing were applied using the LES formulation to simulate B1 flame. The filtered mixture fraction $\tilde{Z}$ transport equation (3.19) was numerically solved, while the mixture fraction variance $Z'^2$ was computed from the equation (3.21) with the standard model’s constant value of $C_v = 0.1$. Both mixing parameters were linked directly to the same flamelet library used for RANS calculations in each grid point. On the other hand, the scalar dissipation rate was computed from the equation (3.22) where $C_x = 2.0$, although different $C_x$ constant values were studied in section 5.4. The LES radial mean and RMS profiles were validated against RANS results and experimental data by (Sevault et al. 2012). In addition, the major species investigated were H$_2$O, H$_2$, CO, and O$_2$. More details about the computational domain, mesh and boundary conditions used by the LES model are discussed below.
5.2.1 Computational Domain and Grid

The computational domain used for the LES simulation with the dimensions is shown in Figure 17. The domain extends from -40 to 150 mm in the axial direction, 97 mm radially, and from 0 to $2\pi$ in the azimuthal direction. Experimentally, the flame was stabilized using the rectangular edged nozzle, therefore; it was fully included in the domain. The burner was placed on $25 \times 25$ cm wind tunnel that accompanies the burned gases with the velocity of 0.5 m/s. The wind tunnel was not included in the domain since the experimental setup ensured no early mixing occurs with air stream below the last location of interest $x/d=20$. The domain was resolved in the axial direction, radial, and azimuthal by $200 \times 140 \times 64$, respectively. The total grid points were 2.1 million cells. The mesh was concentrated in the jet core to resolve the shear layer and stretched axially as shown in Figure 18. The mesh was created using ANSYS mesh 2016.

*Figure 17* Geometry and computational domain for oxy-fuel B1 flame.
5.2.2 Boundary Conditions

The boundary conditions in LES plays an important role in the reproduction of the flow conditions and geometry. For this study, the encountered boundaries used for simulating B1 flame were solid, inflow, and outflow boundaries. The solid boundary was applied for the nozzle walls with no-slip conditions, while the inflow boundary was used for the jet inlet and co-flow inlet. Usually, in LES, the downstream flow calculations are mainly driven by the inflow conditions supplied. Therefore, a careful treatment for the inflow boundary is required. Luckily in our case, the flow was considered fully developed after leaving the nozzle tip. Otherwise, a realistic time varied inlet boundary would have been considered to account for the turbulent fluctuation at the jet inlet. Consequently, it was found that most of the turbulent fluctuation of B1 flame occur due the shear layer effects between the jet stream and the co-flow stream, and not due to the inlet flow conditions. In addition to the velocity supplied at the inlet boundaries, other scalars information were also specified at the inlet. The mixture fraction was specified to be unity for the jet stream and zero for the co-flow, while the mixture fraction variance was set to zero for both inlet streams. On the other hand, the outflow boundary was set to a fixed value for pressure, while zero normal
gradient for all other flow variables. The zero gradient boundary assumes that flow at the outlet is fully developed and no reverse flow occurs. In our case, it was computationally demanding to extend the geometry since we encountered flow re-circulation at the outlet. However, the outlet was placed at 10d far from the area of interest and did not affect the upstream flow calculations. Therefore, the boundary conditions at the outlet were assumed to be zero-gradient for all flow variables, except for the pressure it was set to the atmospheric value.

5.3 Results and Discussion

LES/SLFM was performed for B-1 flame using the conditions listed in Table 2 and the configuration described in section 5.2. The LES results were validated against RANS results and the experimental data of B-1 flame. The mean radial distributions of temperature, mixture fraction, and species mass fraction were predicted, as well as the RMS statistics. Notice that the LES fields were all averaged in the azimuthal direction along with the time averaging operation. The results showed that LES outperformed RANS approach in capturing the flame structure at all axial locations. The upstream radial distribution of temperature in Figure 19 showed that LES accurately predicted the flame mean radial profile and fluctuations compared to RANS model. However, at the location the $x/d=1$, the peak temperature was not captured by either model, although LES was more accurate. The under-prediction of temperature at $x/d =1$ was due to the high scalar dissipation rate predicted at the point, while it is possible that near the nozzle the temperature measurements was not accurate at the location. The radial LES mean and RMS predictions of temperature improved significantly at the location $x/d =3$ and $x/d=5$. Furthermore, the LES predictions of the flame structure kept improving further downstream as illustrated in Figure 20 at the locations $x/d=10$ and $x/d=20$. 
Figure 19 Upstream radial mean profile for temperature at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012), black solid line is RANS/SLFM, and blue dashed line is LES/SLFM.
On the other hand, no major differences were observed for both models in the prediction of the upstream mixing parameters as shown in Figure 21. This indicates that scalar dissipation rate has the most influence on B-1 flame structure and not the mixing parameters; the effect of scalar dissipation will be discussed in section 5.4. However, downstream of the flame at the location $x/d=20$; LES over-predicted the mixture fraction RMS as shown in Figure 22 that led to a slight increase of flame temperature at that location.

**Figure 20** Downstream radial mean profile for temperature and RMS at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012), black solid line is RANS/SLFM, and blue dashed line is LES/SLFM.
Figure 21 Upstream radial mean profile for mixture fraction and RMS at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012), black solid line is RANS/SLFM, and blue dashed line is LES/SLFM.
The mean statistics of major species mass fractions were validated against experimental and RANS data. The mean radial distribution of the species H2O, H2, O2 and CO predicted by LES followed the same trend as the temperature profile predictions discussed earlier. The downstream LES prediction was more accurate than upstream part of the flame as illustrated in Figure 23. That was due to the fact that downstream the flame, scalar dissipation rate effects on the flame structure was minimal. However, H2O mass fraction peak values was not captured accurately in multiple axial locations except for the location x/d=20, while the physical location of peak values were predicted in all locations. That was due to the effect of CO2 that altered some of the reaction pathways as noticed by (Sabia et al. 2015), which was not well represented by GRI 3.0. Therefore, different reaction mechanism for simulating B-1 flame needs to be proposed to account for the CO2 effects on the reaction kinetics.

Figure 22 Downstream radial mean profile for mixture fraction and RMS at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012), black solid line is RANS/ SLFM, and blue dashed line is LES / SLFM.
One of the major limitations of SLFM is that it does not work well with slow chemistry which can affect the species predictions. Therefore, the under-prediction of H2O mean profile could also be due to the transient effects that were not included in the formulation of the flamelet library. However, it would be interesting to study B1 flame using different flamelet models like

\[\text{Figure 23} \text{ Radial mean profile for species mass fractions and RMS at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012). Left plots are for the species O}_2\text{ and CH}_4\text{, while Right plots are for the species H}_2\text{O and H}_2.\]
FPV model or the unsteady flamelet model to come up with a clear conclusion about the effect of chemistry model on the species distributions. Finally, instantaneous and mean contour plots of B-1 flame are listed in Appendix C for temperature, mixture fraction, and species.

5.4 The Influence of Scalar Dissipation Rate

Scalar dissipation rate plays a major role in shaping the structure of non-premixed flames, since it is the variable used to account for the non-equilibrium behavior caused by turbulence. In modeling of turbulent combustion, RANS uses the equation (3.12) in the computation of the mean scalar dissipation rate $\overline{\chi}$. Nevertheless, LES computes the filtered scalar dissipation from the resolved filed using the equation (3.22). Figure 24 showed that RANS, over-predicted the mean scalar dissipation rate four times more than LES approach in all axial locations. That was due to the fact that, LES accurately computed the scalar dissipation from the resolved scales, while RANS computed the mean scalar dissipation from the modeled fields $k$ and $\varepsilon$. Therefore, the flame in RANS calculations got strained more the extinction limit resulting into the under-predictions of temperature as described earlier in section (4.3). However, the mean scalar dissipation rate was reduced dramatically by modifying the constant $C_\chi$ in equation (3.12) as shown in Figure 25, notice that the constant was set to $C_\chi = 0.05$. The modified RANS/SLFM predictions of the mean radial distribution of temperature and H2O mass fraction were improved significantly compare to the standard RANS calculations as illustrated in Figure 26. More calibrations for the RANS/SLFM turbulence and chemistry model’s constants to further improve the predictions. However, the focus of this study to show the effect of scalar dissipation on the predictions of the flame structure. On the other hand, no constant calibrations were required for the LES/SLFM in simulating B-1 flame. Therefore, in the modeling of turbulent combustion, LES became one of the most powerful predictive tools that can accurately capture the flame structure.
Figure 24 Radial mean profile for scalar dissipation rate at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012), black solid line is RANS/ SLFM, and blue dashed line is LES / SLFM.
Figure 25 Modified RANS mean scalar dissipation rate at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012).

Figure 26 Modified RANS upstream radial mean profile for temperature and H2O mass fraction at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012).
LES/SLFM has been performed for B-3 that has higher Reynold number of 18000. Physically, increasing the inlet velocity, increases the mixing rate that takes-over the reaction rate that eventually leads to local extinction of the flame. As results, B-3 flame temperature decreases due to the higher turbulence level compare to the B1 flame, as it was also showing in the experimental

**Figure 27** Modified RANS downstream radial mean profile for temperature and H2O mass fraction at multiple axial locations: red points are experiment data of B-1 from (Sevault et al. 2012).

5.5 LES/SLFM for B-3 Flame

LES/SLFM has been performed for B-3 that has higher Reynold number of 18000. Physically, increasing the inlet velocity, increases the mixing rate that takes-over the reaction rate that eventually leads to local extinction of the flame. As results, B-3 flame temperature decreases due to the higher turbulence level compare to the B1 flame, as it was also showing in the experimental
data (Sevault et al. 2012). The goal was to check if LES/SLFM has the capability to capture the drop in flame temperature that was caused by the increasing turbulence level at the inlet. The results showed that LES/SLFM predicted some level temperature drop as illustrated in Figure 25. However, B-3 flame suffers from a severe local extinction compared to B-1 flame that was not considered in the formulation of the steady flamelet; therefore, the temperature prediction was not accurate. Although, the model was sensitive to the non-equilibrium effects caused by turbulence with the help of the scalar dissipation rate.

Overall, the results showed that LES/SLFM was not appropriate to study the flame B-3 because of the extinction and re-ignition occur in that flame. FPV coupled with LES would be the right model nominee to account for the local extinction occur in B-3 flame. Some work has been established simulating B-3 flame using LES/FPV, where the flamelet library was parametrized against chemical progress variable instead of the scalar dissipation rate. Thus, the progress variable provides the unsteady response of the flame and the non-equilibrium effects. Also, an additional transport equation for progress variable was solved. However, the study is still in progress, and no valuable results can be posted in this piece of work; although a complete study will be proposed later using LES/FPV for B-flames.
Figure 28 Radial mean distributions for B-3 compared to B-1 flame at the location $x/d=5$: red points are experiment data of B-1 from Sevault et al. 2012, yellow symbols are for B-3 Sevault et al. 2012, blue dashed line is LES/SLFM for B-1 and black solid line is LES/SLFM for B-3.
5.6 Conclusion and Future work

LES/SLFM was performed for B-1 flame and compared against RANS/SLFM predictions. In the present study, the LES/SLFM calculations have been successful in predicting the mean and RMS statistics of temperature, mixture fraction, and species mass fractions. The influence of scalar dissipation rate was clearly observed, where LES produced lower scalar dissipation rate than RANS approach that directly affected the flame structure predictions. In LES, the scalar dissipation rate was computed from the resolved scale of the turbulent flow, while in RANS, it was computed from the modeled variables $k$ and $\varepsilon$ that were less accurate. However, RANS predictions were improved by lowering the scalar dissipation rate using different value for the constant $C_{\chi}$. On the other hand, not many discrepancies were found between LES/SLFM and RANS/SLFM for sandia D flame in the prediction of the mean and RMS profiles of temperature and mixture fraction as illustrated by (Clayton & Jones 2008). However, the average radial profile of the species NO and CO was predicted more accurately using LES/SLFM.

LES/SLFM was also used for B-3 flame with higher Reynold number of 18000 compared to 12000 in B-1 flame. The experimental results showed a slight change in flame structure but a higher extinction level compared to B-1 flame. Thus, the adiabatic flame temperature was dropped by about 240K at the location of $x/d=5$, while the LES/SLFM prediction of the temperature drop was only 100K at the same location. That was a consequence of SLFM main formulations that didn’t account for extinction and re-ignition of B-3 flame. Therefore, different flamelet model is recommended for simulating B-3 flame such as FPV/LES, where the flamelet library is parametrized against progress variable instead of scalar dissipation rate.
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APPENDIX A: ADDITIONAL RANS RESULTS FOR SANDIA D FLAME

Sandia D Plots of temperature and other scalars at x/d=60 (red points are experiment data of (Barlow & Frank 2007), solid line is simulation results from RANS/SLFM)
Contour plots for Sandia D:

Contour plot for mean temperature of Sandia D using RANS/SLFM

Contour plot for mean velocity magnitude of Sandia D using RANS/SLFM
APPENDIX B: ADDITIONAL RANS RESULTS FOR B-1 FLAME

B-1 flame plots at x/d=1: (red points are experiment from (Sevault et al. 2012), solid line RANS/SLFM simulation results (Black $\sigma_t=1.6$, Green $\sigma_t=0.85$))
Contour plots for B-1:

Contour plot for mean temperature of B-1 flame using RANS/SLFM

Contour plot for mean velocity magnitude of B-1 flame using RANS/SLFM
APPENDIX C: ADDITIONAL LES RESULTS FOR B-1 FLAME

Instantaneous and mean contour plots of B-1 flame are listed below for temperature, mixture fraction, and species.