Large Eddy Simulation of Premixed and Non-premixed Combustion in a Stagnation Point Reverse Flow Combustor

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Large Eddy Simulation of Premixed and Non-premixed Combustion in a Stagnation Point Reverse Flow Combustor

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To my parents
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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEDICATION</td>
<td>iii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>iv</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>viii</td>
</tr>
<tr>
<td>NOMENCLATURE</td>
<td>xii</td>
</tr>
<tr>
<td>SUMMARY</td>
<td>xvii</td>
</tr>
<tr>
<td>I  INTRODUCTION AND OBJECTIVES</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Motivation and objectives</td>
<td>3</td>
</tr>
<tr>
<td>II  BACKGROUND</td>
<td>7</td>
</tr>
<tr>
<td>2.1 Past studies</td>
<td>7</td>
</tr>
<tr>
<td>2.1.1 Free jet</td>
<td>10</td>
</tr>
<tr>
<td>2.1.2 Confined turbulent jet</td>
<td>11</td>
</tr>
<tr>
<td>2.1.3 Confined/unconfined jet with co-flow</td>
<td>12</td>
</tr>
<tr>
<td>2.1.4 Axisymmetric jet into a dead end chamber</td>
<td>12</td>
</tr>
<tr>
<td>2.1.5 Coaxial jets</td>
<td>12</td>
</tr>
<tr>
<td>2.1.6 Confined coaxial jets</td>
<td>14</td>
</tr>
<tr>
<td>2.1.7 Impinging jet</td>
<td>14</td>
</tr>
<tr>
<td>2.1.8 Entrainment</td>
<td>15</td>
</tr>
<tr>
<td>2.2 Turbulence Combustion Interactions</td>
<td>16</td>
</tr>
<tr>
<td>2.2.1 Combustion regimes</td>
<td>17</td>
</tr>
<tr>
<td>2.2.2 Non-premixed combustion</td>
<td>20</td>
</tr>
<tr>
<td>2.2.3 Modeling</td>
<td>20</td>
</tr>
<tr>
<td>2.2.4 Turbulence chemistry closures</td>
<td>24</td>
</tr>
<tr>
<td>III MATHEMATICAL FORMULATION AND MODELING</td>
<td>29</td>
</tr>
<tr>
<td>3.1 Governing Equations</td>
<td>29</td>
</tr>
<tr>
<td>3.1.1 The Navier-Stokes equations</td>
<td>29</td>
</tr>
<tr>
<td>3.1.2 LES Mathematical Model</td>
<td>31</td>
</tr>
<tr>
<td>3.1.3 SGS Closure for LES equations</td>
<td>33</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>-------</td>
</tr>
<tr>
<td>3.1.4</td>
<td>Localized dynamic kinetic energy model (LDKM)</td>
</tr>
<tr>
<td>3.2</td>
<td>Combustion Modeling</td>
</tr>
<tr>
<td>3.2.1</td>
<td>Eddy Break - Up model (EBU)</td>
</tr>
<tr>
<td>3.2.2</td>
<td>Artificial thickened flame</td>
</tr>
<tr>
<td>3.2.3</td>
<td>Linear-Eddy Mixing model</td>
</tr>
</tbody>
</table>

### IV NUMERICAL IMPLEMENTATION | 43 |
| 4.1 | Finite Volume Scheme | 43 |
| 4.2 | Domain discretization | 45 |
| 4.2.1 | Explicit MacCormack Scheme | 46 |
| 4.2.2 | Numerical Time Step | 48 |
| 4.3 | Boundary Conditions | 48 |
| 4.3.1 | Characteristic boundary conditions | 49 |
| 4.4 | Linear Eddy Mixing Model Implementation | 53 |
| 4.4.1 | The reaction diffusion equation | 54 |
| 4.4.2 | The splicing algorithm | 55 |

### V PROBLEM SETUP | 57 |
| 5.0.3 | SPRF geometry | 57 |
| 5.0.4 | Computational domain | 57 |
| 5.0.5 | Simulated conditions | 58 |
| 5.0.6 | Boundary conditions | 59 |
| 5.0.7 | Grid | 60 |
| 5.0.8 | Chemical kinetics | 67 |
| 5.0.9 | Direct source term estimation | 68 |
| 5.0.10 | Computational costs | 69 |
| 5.0.11 | Numerical issues | 69 |

### VI VALIDATIONS OF PREMIXED CASES | 72 |
| 6.1 | Non-reacting studies | 72 |
| 6.2 | Reactive jet - simple kinetics | 74 |
| 6.2.1 | Time averaged results | 74 |
| 6.2.2 | Instantaneous results | 78 |
# LIST OF FIGURES

1. Schematic diagram of the Stagnation Point Reverse Flow Combustor and an experimental snapshot of a premixed flame .................................... 3
2. Schematic diagram of a confined jet [60] ............................................. 11
4. Premixed turbulent combustion regimes [81] ........................................ 18
5. Premixed turbulent combustion regimes modified for LES applications [84] 20
7. Species field before and after the splicing of the cell (i,j) ....................... 56
8. SPRF geometry ............................................................... 57
9. Computational domain ........................................................................ 58
10. Comparison of Mean and RMS of axial velocity .................................... 61
11. Computational grid ............................................................................ 63
12. FFT of the axial turbulent kinetic energy for the non-reactive jet. This is obtained in the shear layer at an axial distance of 22 mm from the injector and a radial location of 4 mm. ............................................. 64
13. Visualization of coherent structures downstream of the injector using the isosurface of $QU_o^2/D_o^2 = 2 \times 10^9$ ........................................... 65
14. Instantaneous contours of the LDKM coefficients predicted by the LEMLES .......................................................... 66
15. Comparison of the centerline mean axial velocity for the non-reactive jet. 84
16. Comparison of the radial profiles of the mean axial velocity for the non-reactive jet. .............................................................. 84
17. Comparison of the radial profiles of the RMS axial velocity for the non-reactive jet. ............................................................ 85
18. Comparison of averaged heat release rates along a plane passing through the centerline for the reactive jet. The units of heat release in the computations is Joule/sec. ............................................. 85
19. Comparison of the centerline mean axial velocity for the reactive jet. ..... 86
20. Comparison of the radial profiles of the mean axial velocity for the reactive jet. 86
21. Comparison of the radial profiles of the RMS axial velocity for the reactive jet. 87
22. Comparison of the centerline variation of the temperature. Units of temperature is K. .............................................................. 87
23. Comparison of the centerline variation of the $CO_2$ mole fraction. ..... 88
Comparison of the centerline variation of the fuel mole fraction. .......................... 88
Comparison of the radial variation of the fuel mole fraction. .......................... 89
Instantaneous fuel destruction reaction rate contours with the superimposed vorticity contour lines on one half of the plane. .......................... 89
Contours of the instantaneous temperature (K). ........................................ 90
Heat release predictions from LEMLES with simple kinetics (R1) and LEMLES with complex kinetics (R2). Units of the heat release in computations is J/s. ........................................ 91
Contours of the fuel destruction rate. Units of the rate is Kmol/m^3s. ...... 92
Contours of the CO reaction rate. Units of the rate is Kmol/m^3s. ....... 93
Contours of the CO_2 reaction rate. Units of the rate is Kmol/m^3s. ....... 94
Contours of the mean and instantaneous OH mass fraction. ................... 95
Comparison of the centerline mean axial velocity. ............................. 96
Comparison of the radial profiles of the mean axial velocity. ............... 96
Comparison of the radial profiles of the RMS of axial velocity. .............. 97
Instantaneous pressure contours in the non-reacting case. Units in Pascals. 114
Contours of the instantaneous pressure fluctuations in the non-reacting case. Units in Pascals. ........................................ 115
Instantaneous contours of the 3D axial velocity. ................................. 116
Instantaneous contours of the 3D axial vorticity. ................................. 117
Instantaneous contours of the z-direction baroclinic torque. Units in 1/s^2 118
Centerline variation of the size of large scale eddies in the axial direction . 119
Entraining rates ................................................................. 119
Variation of the entrainment coefficient ............................................. 120
Contours of the zero v velocity and zero axial velocity. The boundary between the blue and red colors is the zero v velocity contour. The dark black line is the zero axial velocity contour. The axial distance is provided in mm. ... 120
Radial profiles of the mean v velocity ............................................. 121
Entraining rates ................................................................. 122
Comparison of the radial profiles of the mean v velocity in the R1 and R2 cases 122
Radial profiles of the mean of radial and tangential velocities ............... 123
Radial profiles of the RMS of v and w velocities .................................. 124
Contours of production and dissipation of the turbulent kinetic energy. Units used is $Kg/ms^3$. .......................... 125

Demonstration of the preheating effects in the SPRF combustor .......... 126

Visualization of flame in the near field showing the product entrainment. Isosurface of fuel destruction rate with a value of $1X10^{-4} Kmol/m^3s$ is shown to represent flame surface. The velocity vectors coloured with product mass fraction ($CO_2$) are shown along a plane passing through centerline . 127

Comparison of the species mole fraction along the centerline ............ 128

Radial profiles of the mass fraction of the fuel and air at $x=60$ mm ...... 129

Instantaneous contours of the fuel destruction rate ($Kmol/m^3s$) ........ 129

Operating mode of the SPRF combustor ................................ 130

Contours of instantaneous rates at different instants and different axial locations. Units in $Kmol/m^3$ .......................... 131

Instantaneous strain rate filled contours with contour lines of $CO_2$ formation rate ($Kmol/m^3$). The blue denotes the regions with strain rates less than 100,000 /s and the red color region denotes the regions with strain rates more than 100,000 /s. .................................................. 132

Scatter plots of $CO_2$ formation rate vs. strain rate at different axial locations. Units of $CO_2$ formation rate is $Kmol/m^3s$ and that of strain rate is 1/s . 132

Comparison of the centerline variation of the temperature (K) .......... 133

NO from the thermal and non-thermal pathways and the mean mole fractions of $CO$ and $O_2$. ........................................ 133

Instantaneous contours of $NO$ reaction rates. Units in $Kmol/m^3s$ .... 134

Contours of the mean axial velocity very near to the injector. Units in $m/s$ 144

Centerline variation of mixture fraction. ............................... 145

Instantaneous contours of the axial velocity. Units in $m/s.$ .............. 146

Flame location in experiments [34] and different LES sub-grid closures. Heat release is used to represent the flame location except in SFLES where temperature contours are used. The units of computed heat release is $J/s$ .... 147

Comparison of the centerline mean axial velocity. ....................... 147

Comparison of the radial profiles of the mean axial velocity. .......... 148

Comparison of the radial profiles of the RMS axial velocity. .......... 148

Comparison of temperature along the centerline. .......................... 149

Comparison of carbon dioxide mole fraction along the centerline. .... 149
Instantaneous reaction rates in the premixed and non-premixed modes. Units in \( \text{Kmol/m}^3\text{s} \) ................................. 150

Variation of the reaction rates along the centerline. The rates are averaged over the entire cross section at every axial location. Units of the rate is \( \text{Kmol/s} \) 151

Scatter plots of reaction rate vs. temperature. Units of reaction rate is \( \text{Kmol/m}^3\text{s} \) and temperature is \( \text{K} \) ................................. 151

Filled contours of the scalar dissipation rate with contour line of the fuel destruction rate. The units of scalar dissipation is \( 1/\text{s} \) ................................. 152

Isocontour of the instantaneous reaction rate colored with F.I.. Color red denotes +ve F.I. and color blue denotes -ve F.I. ................................. 152

Scatter plot of fuel destruction rate vs mixture fraction. Units of fuel destruction rate is \( \text{Kmol/m}^3\text{s} \) ................................................................. 153

Variation of the % of the heat release with the mixture fraction. .......... 153

Entrainment rates for the reacting cases. ................................. 154

Centerline variation of the products mole fraction. ................................. 155

Radial profiles of \( O_2 \) ................................................................. 155

Dilution in the non-premixed mode. ................................................................. 156
**NOMENCLATURE**

**Roman Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{EBU}$</td>
<td>model coefficient for the Eddy Break-Up model</td>
</tr>
<tr>
<td>$C_e$</td>
<td>model coefficient for subgrid dissipation</td>
</tr>
<tr>
<td>$C_\lambda$</td>
<td>scalar diffusivity</td>
</tr>
<tr>
<td>$C_\nu$</td>
<td>model coefficient for turbulent viscosity</td>
</tr>
<tr>
<td>$c$</td>
<td>speed of sound</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure per unit mass</td>
</tr>
<tr>
<td>$c_v$</td>
<td>specific heat at constant volume per unit mass</td>
</tr>
<tr>
<td>$D$</td>
<td>mass diffusivity</td>
</tr>
<tr>
<td>$D^{sgs}$</td>
<td>dissipation of turbulent kinetic energy</td>
</tr>
<tr>
<td>$Da$</td>
<td>Damkohler number</td>
</tr>
<tr>
<td>$E$</td>
<td>Efficiency function in Thickened Flame model</td>
</tr>
<tr>
<td>$E_a$</td>
<td>activation energy</td>
</tr>
<tr>
<td>$e$</td>
<td>internal energy per unit mass</td>
</tr>
<tr>
<td>$F$</td>
<td>Flame thickening factor</td>
</tr>
<tr>
<td>$F$</td>
<td>flux vector in $x$ direction</td>
</tr>
<tr>
<td>$G$</td>
<td>flux vector in $y$ direction</td>
</tr>
<tr>
<td>$H$</td>
<td>flux vector in $z$ direction</td>
</tr>
<tr>
<td>$H_i$</td>
<td>total enthalpy per unit mass</td>
</tr>
<tr>
<td>$h$</td>
<td>enthalpy flux</td>
</tr>
<tr>
<td>$i, j, k$</td>
<td>specific enthalpy per unit mass</td>
</tr>
<tr>
<td>$i, j, k$</td>
<td>computational grid indices</td>
</tr>
<tr>
<td>$J$</td>
<td>Jacobian of the coordinate system transformation</td>
</tr>
<tr>
<td>$k$</td>
<td>turbulent kinetic energy</td>
</tr>
<tr>
<td>$k^{sgs}$</td>
<td>sub-grid turbulent kinetic energy</td>
</tr>
</tbody>
</table>
\begin{itemize}
  \item \textit{Ka} \quad \text{Karlovitz number}
  \item \textit{ℓ} \quad \text{integral length scale}
  \item \textit{l}_f \quad \text{flame thickness}
  \item \textit{l}_G \quad \text{Gibson length scale}
  \item \textit{l}_m \quad \text{mixing length scale}
  \item \textit{l}_δ \quad \text{thickness of the flame inner layer}
  \item \textit{Le} \quad \text{Lewis number}
  \item \textit{MW} \quad \text{molecular weight}
  \item \textit{N} \quad \text{total number of species}
  \item \textit{P} \quad \text{production of turbulent kinetic energy}
  \item \textit{p} \quad \text{pressure}
  \item \textit{Pr} \quad \text{Prandtl number}
  \item \textit{Q}, \textit{Q}' \quad \text{state vector}
  \item \textit{q}_i \quad \text{heat flux}
  \item \textit{Re} \quad \text{Reynolds number}
  \item \textit{R}_u \quad \text{universal gas constant}
  \item \textit{r} \quad \text{spatial position}
  \item \textit{S} \quad \text{rate of strain}
  \item \textit{S}_L \quad \text{laminar flame speed}
  \item \textit{T} \quad \text{temperature}
  \item \textit{t} \quad \text{time}
  \item \textit{u}, \textit{v}, \textit{w}, \textit{u}_i \quad \text{Cartesian velocity vector components}
  \item \textit{u}' \quad \text{\textit{rms} velocity}
  \item \textit{v}' \quad \text{turbulent intensity}
  \item \textit{u}'_{sgs} \quad \text{subgrid scale turbulence intensity}
  \item \textit{V} \quad \text{volume}
  \item \textit{V}_{i,m} \quad \text{diffusion velocity of species \textit{m}}
  \item \textit{x}, \textit{y}, \textit{z} \quad \text{Cartesian coordinate directions}
  \item \textit{X} \quad \text{mole fraction}
\end{itemize}
$Y$ mass fraction

$Y_{i,m}$ flux of species $m$

**Greek Symbols**

- $\alpha$ thermal diffusivity
- $\gamma$ ratio of specific heats
- $\Delta$ grid size
- $\delta_{ij}$ Kronecker delta
- $\Delta h_f'$ specific heat
- $\Delta h_f$ enthalpy of formation per unit mass
- $\phi$ equivalence ratio
- $\Phi_{i,m}$ convective mass flux of species $m$
- $\eta$ Kolmogorov length scale
- $\theta_{i,m}$ diffusive flux of species $m$
- $\kappa$ thermal conductivity
- $\lambda$ stirring frequency
- $\mu$ dynamic viscosity
- $\nu$ kinematic viscosity
- $\nu_m$ stoichiometric coefficient
- $\rho$ density
- $\tau_{ij}$ viscous stress tensor
- $\sigma$ wave reflection coefficient
- $\sigma_{ij}$ viscous work
- $\xi$, $\eta$, $\zeta$ spatial directions in computational space
- $\Upsilon_{s gs}$ species-temperature correlation term
- $\dot{\omega}$ reaction rate per unit volume

**Subscripts**
e.g.s cm-gram-second measurement system  
i, j, k Cartesian tensor indices or species indices  
k species index  
L laminar  
m chemical index  
n time step index  
t, T turbulent quantity  
u unburned  
∞ quantity at infinity downstream

### Superscripts

<table>
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<tr>
<td>0</td>
<td>reference quantity</td>
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<tr>
<td>LEM</td>
<td>quantity at the LEM level</td>
</tr>
<tr>
<td>sgs</td>
<td>subgrid scale</td>
</tr>
<tr>
<td>stir</td>
<td>stirring</td>
</tr>
<tr>
<td>test</td>
<td>test filter scale</td>
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### Other Symbols

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<thead>
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<th>Symbol</th>
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<tr>
<td>∂</td>
<td>partial derivative operator</td>
</tr>
<tr>
<td>∇</td>
<td>gradient operator</td>
</tr>
<tr>
<td>∇.</td>
<td>divergence operator</td>
</tr>
<tr>
<td>Σ</td>
<td>summation operator</td>
</tr>
<tr>
<td>Δ</td>
<td>difference operator</td>
</tr>
<tr>
<td>~</td>
<td>Favre spatial filter</td>
</tr>
<tr>
<td>^</td>
<td>test filter</td>
</tr>
<tr>
<td>-</td>
<td>space average</td>
</tr>
<tr>
<td>′, ″</td>
<td>fluctuating quantity</td>
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**Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>ANN</td>
<td>Artificial Neural Network</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy number</td>
</tr>
<tr>
<td>CPU</td>
<td>Central Processing Unit</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>DSTE</td>
<td>Direct Source Term Estimation</td>
</tr>
<tr>
<td>DVODE</td>
<td>Double precision Variable Coefficients Ordinary Differential Equations solver</td>
</tr>
<tr>
<td>EBU</td>
<td>Eddy Break-Up model</td>
</tr>
<tr>
<td>EBULES</td>
<td>Eddy Break-Up model approach with Large Eddy Simulation</td>
</tr>
<tr>
<td>LDKM</td>
<td>Localized Dynamic $k$-equation Model</td>
</tr>
<tr>
<td>LEM</td>
<td>Linear Eddy Mixing model</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>LEMLES</td>
<td>Linear Eddy Mixing model with Large Eddy Simulation</td>
</tr>
<tr>
<td>LODI</td>
<td>Local One-Dimensional Inviscid</td>
</tr>
<tr>
<td>MPI</td>
<td>Message Passing Interface</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary Differential Equation</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Distribution Function</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds Averaged Navier - Stokes</td>
</tr>
<tr>
<td>TKE</td>
<td>Turbulent Kinetic Energy</td>
</tr>
<tr>
<td>RMS</td>
<td>Root Mean Square, variance</td>
</tr>
</tbody>
</table>
A new combustor referred to as Stagnation Point Reverse Flow (SPRF) combustor has been developed at Georgia Tech to meet the increasingly stringent emission regulations. The combustor incorporates a novel design to meet the conflicting requirements of low pollution and high stability in both premixed and non-premixed modes. The objective of this thesis work is to perform Large Eddy Simulations (LES) on this lab-scale combustor and elucidate the underlying physics that has resulted in its excellent performance. To achieve this, numerical simulations have been performed in both the premixed and non-premixed combustion modes, and velocity field, species field, entrainment characteristics, flame structure, emissions, and mixing characteristics have been analyzed.

Simulations have been carried out first for a non-reactive case to resolve relevant fluid mechanics without heat release by the computational grid. The computed mean and RMS quantities in the non-reacting case compared well with the experimental data. Next, the simulations were extended for the premixed reactive case by employing different sub-grid scale combustion chemistry closures: Eddy Break Up (EBU), Artificially Thickened Flame (TF) and Linear Eddy Mixing (LEM) models. Results from the EBU and TF models exhibit reasonable agreement with the experimental velocity field. However, the computed thermal and species fields have noticeable discrepancies. Only LEM with LES (LEMLES), which is an advanced scalar approach, has been able to accurately predict both the velocity and species fields. Scalar mixing plays an important role in combustion, and this is solved directly at the sub-grid scales in LEM. As a result, LEM accurately predicts the scalar fields. Due to the two way coupling between the super-grid and sub-grid quantities, the velocity predictions also compare very well with the experiments. In other approaches, the sub-grid effects have been either modeled using conventional approaches (EBU) or need some *ad hoc* adjustments to account these effects accurately (TF).
The results from LEMLES, using a reduced chemical mechanism, have been analyzed in the premixed mode. The results show that mass entrainment occurs along the shear layer in the combustor. The entrained mass carries products into the reactant stream and provides reactant preheating. Thus, product entrainment enhances the reaction rates and help stabilize the flame even at very lean conditions. These products have been shown to enter into the flame through local extinction zones present on the flame surface. The flame structure has been further analyzed, and the combustion mode was found to be primarily in thin reaction zones. Closer to the injector, there are isolated regions, where the combustion mode is in broken reaction zones, while the downstream flame structure is closer to a flamelet regime. The emissions in the combustor have been studied using simple global mechanisms for \( NO_x \). Computations have shown extremely low \( NO_x \) values, comparable to the measured emissions. These low emissions have been shown to be primarily due to the low temperatures in the combustor. LEMLES computations have also been performed with a detailed chemistry to capture more accurate flame structure. The flame in the detailed chemistry case shows more extinction zones close to the injector than that in the reduced chemical mechanism.

The LEMLES approach has also been used to resolve the combustion mode in the non-premixed case. The studies have indicated that the mixing of the fuel and air close to the injector controls the combustion process. The predictions in the near field have been shown to be very sensitive to the inflow conditions. Analysis has shown that the fuel and air mixing occurs to lean proportions in the combustor before any burning takes place. The flame structure in the non-premixed mode was very similar to the premixed mode. Along with the fuel air mixing, the products also mixed with the reactants and provided the preheating effects to stabilize the flame in the downstream region of the combustor.
CHAPTER I

INTRODUCTION AND OBJECTIVES

1.1 Introduction

Combustion of hydrocarbon fossil fuels provides most of the world’s energy [94]. To date, it is the major source of energy available to mankind. This type of energy is stored in the form of chemical bonds of hydrocarbons (e.g. oil, gasoline, diesel fuel), and is used for transportation (land, sea, air), electricity generation, heating buildings, and industrial processes [116]. This is the beneficial side of combustion. The downside is that it pollutes the environment. Some of the major pollutants produced by hydrocarbon combustion are unburnt and partially burnt hydrocarbons, nitrogen oxides ($NO$ and $NO_2$), carbon monoxide, sulfur oxides, and particulate matter in various forms. These pollutants can cause health problems, smog, acid rain, global warming, and ozone depletion. As a result, stringent regulations have been imposed by government agencies (e.g., EPA, NASA) on emission levels. These regulations have been pushing the combustion research to optimize combustor designs for reduced emissions on both land and air based combustors. In addition, due to the depletion of oil resources, there is always need to improve performance, lower costs and at the same time operate without sacrificing reliability.

$NO_x$ can be formed through different pathways during combustion [72]. $NO_x$ formed during high temperature, which is known as thermal $NO_x$ has been found to be a prominent regulated emission in practical combustors. High amounts of $NO_x$ are typically seen in mixtures that are reacting under stoichiometric (the amount of air needed to completely burn the fuel) conditions due to high temperature prevalent in such a system. Hence, a popular method used to reduce $NO_x$, especially for premixed systems, is to burn under fuel lean conditions, where there is an excess of oxidizer present in the combustor. The leaner the mixture, lower the temperature, and hence, lower the generation of NOx. However, there is a limit to these lean conditions. It is well known that the very lean premixed operation
can impact the static stability through lean blow out phenomenon. Furthermore, injecting premixed fuel and air can lead to a flashback or autoignition in the premixer, which is not desirable. Another means of achieving low $NO_x$ is using flue gas recirculation (FGR) [6]. It involves addition of the inert low temperature products of combustion to air or the fuel prior to combustion. FGR reduces NOx by reducing flame temperatures and local oxygen concentrations in the flame zone.

A recent development that has demonstrated lower emissions and stable combustion over a range of furnace applications is the high-temperature air combustion (HITAC) [115, 43, 37, 36] or flameless oxidation [123], which is used in connection with the exhaust gas recirculation (EGR) concept. In this technology, a part of the hot combustion products is recirculated into preheated combustion air to reduce the oxygen concentration. Both high efficient combustion and low $NO_x$ emissions are achieved in HITAC technology.

The Stagnation Point Reverse Flow (SPRF) combustor [77] is another combustor which uses some of the above concepts, and has been investigated computationally within the context of the current study. A schematic sketch of the combustor along with a snap shot of the flame during the experiments are shown in Fig. 1. The combustor consists of an injector tube through which fuel and air are injected into a cylindrical chamber that is open at one end and closed at the other. The reactants burn as they flow towards stagnation plate. The inflow and outflow are located on the same side of the combustor, thus, the products are able to interact with the incoming reactants as they exit the combustor. The configuration has been shown to operate stably with ultra low $NO_x$ emissions in both the premixed and non-premixed modes of combustion over a wide range of operating conditions [34, 22, 11]. It should be noted that the SPRF design exhibits a complex flow field due to the existence of flow confinement, flow stagnation, coaxial jets and flow of two opposing streams that are coupled to each other. Hence, a detailed description of the flow and the combustion process occurring inside the combustor using computations is a challenging task. Furthermore, the turbulence-combustion interaction occurring within the combustor is far more complex than that occurring within classical combustors. Thus, state-of-the-art computational models are needed to resolve the complex flow physics under various
1.2 Motivation and objectives

The purpose of this current investigation is to use numerical simulations to predict the flow and the combustion phenomenon in both the premixed and non-premixed modes in the SPRF configuration. SPRF incorporates a coaxial jet flow into a confined tube with a stagnation end plate. The flow also includes the interaction of the ingoing jet with the exhaust jet. A reverse flow combustor [125] shows resemblance to this combustor design with the difference that the ingoing and exhaust jets are decoupled. There were no previous detailed numerical simulations of such combustor designs. Even for non-reacting conditions, there is one numerical study by Amano [4], with a design similar to the SPRF. This study addressed numerically the flow of a turbulent, axisymmetric jet into a cylindrical tube closed at the end opposite to the injection plane with a plate. The flow features are studied for different distances between the injection plane and the end wall.

Thus, no previous computational studies exist that has resolved the flow and the combustion in a configuration such as SPRF. Hence, the primary contribution of this thesis is the description of the flow and the combustion phenomenon in both the premixed and
non-premixed modes in the SPRF configuration.

Large Eddy Simulations (LES) have been used as the numerical tool in the current work. Although LES is computationally more expensive than the traditional Reynolds Averaged Navier Stokes (RANS) approach, its advantage is that the large-scales, which contain most of the turbulent kinetic energy and control the dynamics of the turbulence, are directly resolved [83]. As a result, LES solves the unsteady and intermittent behaviour of the large scale eddies that are responsible for mixing [74]. Hence, LES is fast becoming the design tool to model combustors. It has been applied to a number of combustor applications in predicting the emissions [26], premixed combustion [17, 100], non-premixed combustion [68, 15], flame blowoff [108], combustion instabilities [5, 111, 103] and practical engine combustion [23].

Even though advances in the computational resources are making LES suitable for turbulent combustion applications, its full potential as a design tool has not yet been developed. The main reason for this is that even though the major part of the energy containing eddies are directly solved in LES, combustion is predominantly a molecular phenomenon, and a sub-grid model is still needed to model this sub-grid scale phenomenon. A number of such sub-grid closures (e.g., eddy break up closure [32], artificial thickened flames [21], steady [80] and unsteady flamelet models [64]) are available in the literature. However, with the exception of filtered probability density (FPDF) [88] and Linear Eddy Mixing (LEM) [49, 69] approach, the models either have specific applicabilities or need ad hoc adjustments. Hence, there is a need to establish a numerical approach that requires no user input and can capture flow-flame features in very different operating modes without any model adjustments. This forms the secondary objective of this thesis.

The following tasks are defined to meet the above objectives.

- **Task 1**: LES of non-reactive flow in the premixed flow configuration.
  The non-reacting studies are first performed to validate the numerical approach as well as to examine the flow features in the SPRF setup. The results are be used to distinguish the flow features in this configuration with that of conventional flows.
Task 2: LES of reactive premixed case using different sub-grid closures with a reduced mechanism.

The reacting studies are performed using different turbulent chemistry closures that have been established in the literature. The results from all the approaches are validated with the experiments. Then the best approach (LEM) is used to investigate the premixed combustion mode. In particular, the studies examine how heat release effects the interaction of the forward and return flow jets. The combustion characteristics, such as heat release, flame structure, are analyzed to determine the operation mode. Emissions are evaluated in the simulations.

Task 3: LES of reactive premixed case using a multi-step chemistry

A detailed chemistry case is studied in the premixed case. The results are compared to the simple chemistry case and the differences and similarities of the flame structure are identified.

Task 4: LES of reactive non-premixed case.

The LEM model is used to simulate the non-premixed combustion mode without making any changes to the earlier version. The results are used to understand the flame structure in this mode. The differences in the mixing characteristics between the premixed and non-premixed mode are analyzed.

The thesis is organized as follows:

1. Chapter 2 provides background on the subject of interest. It provides a detailed discussion of the past studies that have led to the novel design. This will be followed with a literature study of various types of jet flows that are present in the SPRF setup. Also, this chapter provides a background on the numerical issues in turbulent combustion.

2. Chapter 3 gives the details about the mathematical formulation and different sub-grid closure models used in the simulations.

3. Chapter 4 explains the numerical method employed in solving the governing equations.
It also provides the numerical implementation of the boundary conditions and the Linear Eddy Mixing (LEM) model in the simulations.

4. Chapter 5 describes the problem setup, where the description of the experimental setup, the computational domain, the computational grid, and the timing studies are presented.

5. Chapter 6 shows the validations of the simulations in the non-reacting and reacting premixed cases. The reacting studies include EBULES, TFLES and LEMLES calculations.

6. Chapter 7 describes the flow and combustion features in the premixed mode

7. Chapter 8 presents the results in the reacting non-premixed mode with emphasis on the differences between the premixed and the non-premixed operating modes.

8. Chapter 9 provides the conclusions and some suggestions for future research.
This chapter provides a brief background on the issues that are concerned with the design of the combustor as well as the computational issues related with combustor modeling. The first part deals with the past studies that have paved the path for SPRF design. In the later part of the chapter, experimental and computational studies that are connected to some of the flow features present in the SPRF configuration are presented. Finally, the modeling issues related to turbulent combustion in both premixed and non-premixed mode are discussed.

2.1 Past studies

Due to the new stringent regulations on pollutant emissions and requirement for high performance, the interest in low emission combustion is continuously increasing. A number of new designs are being proposed to reduce combustor emissions. One prominent emission in the form of oxides of Nitrogen is $NO_x$. $NO_x$ is produced through different mechanisms. However, for most gas turbine combustors, $NO_x$ produced through high temperatures (or thermal $NO_x$) is believed to be the dominant mechanism [57]. Hence, most of the strategies have been developed around this idea of reducing the peak temperature inside the combustor. Some of these methods include:

1. Dilution: Diluting the combustion products with diluents such as $CO_2$, $N_2$ can lower the temperature in the combustor and reduce $NO_x$.

2. Premixed lean combustion: In a lean premixed system, the fuel and excess oxidizer mix upstream of the combustor. This lowers the temperature and hence thermal $NO_x$.

3. Catalytic combustion: In catalytic combustors, lean systems are supported by the catalytic reactor bed to burn very lean fuel air mixtures.
4. Post combustion: In this method, $NO_x$ from the exhaust of the combustor is made to react with ammonia and selective catalytic reduction (SCR) catalyst to produce molecular nitrogen. Thus, $NO_x$ entering into the atmosphere is reduced. However, these systems poses many disadvantages in the form of pressure drop due to the addition of external devices and addition of new pollutant in the form of ammonia.

Lean systems are the subject of interest in this work. The demand for lower emissions will push the systems towards more leaner. But these systems possess problems such as unexpected blow out (where the flame can not stay inside the combustor) and damage the system due to acoustic vibrations. Hence, the combustor design should be such that it can ensure the flame inside the combustor under all operating conditions. To stabilize the flame, appropriate flow conditions along with proper chemical mixtures must be present in the combustor. The flame must be anchored in a region where the velocity of the incoming reactant mixture is low. These low velocities provide sufficient time for the reactants to ignite and start combustion. For stability, the flow velocity must balance the speed of the flame that is approaching the reactants. For example, in a Bunsen burner, the flame is anchored near the burner’s rim due to the balance of low velocity near the rim with the flame speed. The flame here is sustained due to the molecular conduction of heat and molecular diffusion of radicals into the approaching reactants. The same fundamentals are also used to hold the flame in a gas turbine. However, due to high inflow velocities, different flame holding mechanisms are being incorporated. In most of the cases, flame anchoring is accomplished by the use of one or more swirlers that create recirculation regions of low velocities. These regions hold the flame due to the recirculation of hot combustion products into reacting pockets that continuously ignite the incoming reactants [113]. Low velocity regions can also be created by introducing bluff bodies or V-shaped gutters. Again, the mechanism for continuous burning is the same as that with the swirlers.

One recent development in combustion systems that reduce $NO_x$ is the high temperature air combustion [37] or flameless combustion [123]. This technology combines high velocity fuel and air jets, high temperature air and hot product recirculation. The high temperature air is obtained by preheating the air with exhaust gases from an external furnace or reactor.
In this technology, a part of the combustion products is recirculated into the incoming hot combustion air. This leads to low oxygen concentrations (dilution effects) and a reduction of the flame temperature compared to conventional burners. These flames with highly preheated air are shown to be significantly more stable and homogeneous when compared to room temperature air combustion. Under certain conditions of the high temperature air combustion, no visible flame is observed, hence, the name flameless combustion. Low levels of \( NO_x \) along with negligible levels of \( CO \) and unburned hydrocarbons are obtained in this system. However, it has its own drawbacks. The system requires high velocity fuel and air jets to ensure the entrainment of reactants with hot products. And this large kinetic energy is dissipated inside the combustor leading to large pressure losses. In addition, since the mixing of reactants with large amounts of exhaust gases is needed, the amount of fuel burned per unit volume per second is less. Hence a combustor of large volume is needed to generate high power density. This requirement makes this system unsuitable for aircraft engine applications where compactness is highly preferred.

Another combustor that has been widely studied is the jet stirred reactor (JSR) [110]. In this system, the combustion process is mainly mixing controlled. In JSR, a lean premixed mixture of the fuel and oxidizer is injected along one or more high velocity jets into a relatively small combustor volume. The high momentum of the incoming jets produces very fast mixing of the incoming reactants with the hot combustion products, and burns the gases within the combustor. The fast mixing also results in a very rapid ignition and combustion that is nearly uniformly distributed throughout the combustor volume. JSR has been extensively used to study the effects of different parameters on \( NO_x \). \( NO_x \) formation is shown to be a result of many competing factors such as fuel type, equivalence ratio, the degree of fuel air mixing, pressure, reactants temperature, flow velocity, mixing characteristics, residence time inside the flame and post-flame zones.

Some of the ideas from the above combustion systems can be summarized as follows.

- Incorporating high velocity fuel and air jet inside a small compact combustor improves mixing between the fuel and air and between the reactants and combustion products
• Burning with high temperature air provides a stable combustion at lean conditions

• Burning in diluted oxygen gives a low peak temperature in the flame zone. This can be achieved with a high recirculation of the hot products into the reactant stream

The novel SPRF combustor incorporates some of the above ideas. A schematic sketch of the combustor is shown in Figure 1. The combustor operates in both premixed and non-premixed modes. The combustor design also provides the heating of the premixed/air jet in premixed/non-premixed mode due to the flow of products over the injector. Hence, air gets heated to high temperatures before it enters into the combustor. Also, there is an internal recirculation of the products into the reactants, which dilutes the combustion air. The reactants are injected into the combustor at high velocities.

The design of the SPRF configuration encompasses the following flow features:

• confined turbulent jets

• coaxial turbulent jets

• stagnation region

• jet interacting with a reverse co-flow jet

• jet entrainment

All these features are simultaneously present in the configuration. In addition, heat release also alters the flow features in this configuration. There are no previous studies that incorporated all the above features. The studies on an axisymmetric jet issuing into an axisymmetric dead end chamber, performed by Abramovich [1], are very similar to that of the SPRF setup. A review of these studies along with studies on confined jets, coaxial jets, stagnation regions and entrainment is provided here.

2.1.1 Free jet

Extensive literature can be found on free turbulent jets. The main characteristics of free jets are the conservation of axial momentum and the dynamic similarity of velocity profiles
at different axial locations downstream of the potential core [30]. Based on this, the velocity of the jet decays along the centerline as a function of inverse of the axial distance \(1/x\).

2.1.2 Confined turbulent jet

Confining a turbulent jet inside a tube can alter the behavior of the jet. A schematic sketch [60] of a confined jet flow is shown in figure 2. The jet development in the axial direction can be divided into three main regions. The first region is from the injector to the potential core (=5d). The second region is similar to that of the self-preserving region of a free turbulent jet. The third region starts at the point where the jet width is equal to the confining tube diameter. Experiments with confined jets have showed that a generic equation can be derived in the second region due to the self-preserving nature. The centerline velocity decay is shown to be a function of the axial distance as well as the ratio of the injector tube diameter \(d\) to the confined tube diameter \(D\).

\[
\frac{u}{U_0} = C_1 \frac{d}{x} + f\left(\frac{d}{D}\right) \tag{1}
\]

where, \(U_0\) is the velocity at the injector and \(C_1 = 6.3\). Liu et al. [60] approximated the function \(f\left(\frac{d}{D}\right)\) to be a polynomial relation. Neglecting the higher order terms, they arrived at a relation which is valid for a free jet as well as for the second region of a confined jet.

\[
\frac{u}{U_0} = 6.3 \frac{d}{x} - 1.4 \frac{d}{D} \tag{2}
\]
The above relation shows that the confinement leads to a lower decay of the centerline velocity when compared to a free jet.

2.1.3 Confined/unconfined jet with co-flow

The co-flowing streams were also shown to have an effect on the flow field in confined jets. The velocity of the co-flow are typically much lower than that of the main jet. Borean et al. [12] showed that a confined jet behaved like a free jet in the presence of a weak co-flow, whereas significant changes were observed in the absence of the co-flow. A strong co-flow changed the centerline velocity decay to $x^{-2/3}$ instead of $x$ [91]. In these studies, the co-flow is in the same direction as the central jet.

2.1.4 Axisymmetric jet into a dead end chamber

Abramovich [1] developed theoretical models for jets issuing into long dead end chambers. He conducted experiments with two sets of configurations. One set was where the jet does not penetrate far enough to impinge on the end plate, while in the second, the jet impinges on the end plate. In the case where the jet does not impinge on the end plate, only the jet center reaches the farthest point. The fluid at the outer edge of the jet reverses its direction before reaching the farthest point. As the jet spreads, the mass flow in the streamwise direction increases due to entrainment. Mass conservation ensures that whatever enters into the chamber must leave. Hence the net mass flux at each cross section is found to be zero. Similar experimental studies were also conducted by Eckmann et al. [25] in the laminar regime. The penetration length was invariant with the Reynolds number in the laminar region while the turbulent models by Abramovich [1] shows that penetration length is is invariant with the Reynolds number.

2.1.5 Coaxial jets

Coaxial jets are used in various industrial devices due to their efficient mixing of jets in combustion applications. They are composed of an inner jet of diameter $D_1$ issuing with velocity $U_1$ and density $\rho_1$, and an larger outer jet of diameter $D_2$ issuing with velocity $U_2$ and density $\rho_2$. One of the important parameters that characterize the coaxial jet dynamics
is the ratio between the outer jet momentum flux to the inner jet momentum flux. Rehab et al. [118, 92] studied extensively the near field dynamics of the constant density coaxial flow, in which case, the critical parameter is the velocity ratio, \( r_u = U_2/U_1 \). In a pure annular jet (in which \( U_1 = 0 \)), the flow in the near field is characterized by the presence of a recirculation near the jet axis [55]. Hence, if an inner jet is issued into the chamber with low velocity, a recirculation bubble can still be present near the jet axis. As the inner jet velocity is increased, for some \( r_u = r_{uc} \gg 1 \), the recirculation bubble was observed in the experiments [92]. Under these conditions, regions with backflow were observed near the jet axis. And the other limiting case, which is of interest is the single round jet (assuming zero lip thickness between the outer and inner jets) case, where \( r_u = 1 \). In such a case, recirculation zones are not possible. Hence, there exists a range of the \( r_u \) values which separate the two main flow regimes; without recirculation bubble for \( 1 < r_u < r_{uc} \) and with recirculation bubble for \( r_u > r_{uc} \). The occurrence of the recirculation bubble is explained by Rehab et al. [92]. When the critical velocity is beyond the \( r_{uc} \), the outer jet begins to penetrate upstream on the inner jet axis. This entrainment process creates a radial pressure jump between the two jets. Experiments showed that as long as the incident kinetic pressure is larger than radial pressure jump, the inner jet is able to prevent the formation of the recirculating flow. When \( r_u \) is increased beyond \( r_{uc} \), the pressure jump may exceed the kinetic pressure and reverse flow is possible. Many parameters affect the value of \( r_{uc} \), i.e, onset of the recirculation bubble. Rehab et al. [93] showed that the \( r_{uc} \) depends on the annular gap width, the exit velocity profile and the retraction of inner injector with respect to the external nozzle.

It is of fundamental interest to understand the importance of the recirculation bubble on the mixing behavior of the coaxial jets in the near field. A passive scalar mixing problem was studied using Direct Numerical Simulations (DNS) by Balarac et al. [7] in free round coaxial jets. Species are seeded in the outer and inner jets and mixing efficiency is evaluated using mixture fraction. The results showed that the recirculation bubble is a region with a significant production of intense streamwise vortices. These streamwise vortices appear very early in the inner shear layer and significantly increase the turbulent mixing activity.
Thus, recirculation bubble plays a considerable role in the mixedness of the outer jet with the inner jet. The streamwise vortices are also observed in the cases with out recirculation bubble that can aid in the near field mixing of the coaxial jets. These mixing aspects were quantified by Vilermaux [118] using a dilution length, defined as the axial distance by which the concentration of central jet reduces to a specified level. Under the condition that \( r_u < r_{uc} \), the dilution length is estimated as a function of \( r_u \) and inner jet diameter.

\[
L_d = D_1 r_u C_0 / C_s
\]

where \( C_0 \) is the central jet concentration and \( C_s \) is the specified level of dilution. The above relation can be extended to jets with different densities by replacing \( r_u \) with square root of the momentum ratio.

2.1.6 Confined coaxial jets

There are not any studies that address the recirculation bubble in the confined coaxial jets. A study by Lima and Palma [59] showed that confinement played no role in the onset of the region with axial negative velocity. The study showed that the confined coaxial jet behaved like a non-confined coaxial jets with respect to the onset of the recirculation bubble.

2.1.7 Impinging jet

There are some experimental studies in the literature on confined jet flows impinging on stagnation plates. The main application of these kind of jets is in industries that require high rates of heat and mass transfer. The flow characteristics are found to be very sensitive to the spacing between the injector and the stagnation plate (\( H \)). In the impinging jet flow, as shown in Figure 3, there are three regions of distinct flow named as free jet region, wall jet region and impinging region [8]. In the free jet region, the flow is not influenced by the stagnation plate and the dominant velocity is axial. The wall jet region is where the dominant velocity component is radial. The impingement region lies between the other two and characterized by the significant changes in flow direction. Typically, in these studies, \( H/D \) is maintained very low (below 5). However, in the SPRF configuration, the stagnation plate is located at about 25 annular jet diameters from the injector. Hence, it
can be expected that most of the flow regime in SPRF will be in free jet region. Not only the impinging plate in SPRF is located far away, but also it is located within the confining walls of the system.

2.1.8 Entrainment

Entrainment is defined as the radial inward flux of an ambient fluid drawn into a jet. It is usually given by $e = \dot{m}_e / \dot{m}_o$ where $\dot{m}_e = \int_0^R 2\rho \bar{u} \pi r dr$. Here $\dot{m}_o$ is the inflow flow rate and $R$ is defined as the location at which the velocity $u$ goes to zero. The entrainment rate controls mixing of the central jet with the ambient fluid. In the coaxial jet configurations found in many non-premixed combustors, the entrainment rate plays a critical role in mixing the fuel and air, and consequently affects the residence times and reaction rates. Therefore, the study of entrainment of jets is of fundamental interest for pollutant formation and soot formation in a reacting jet [20].

The entrainment into a turbulent jet flame was investigated by various earlier works [9, 16, 38]. A summary of these studies is that the local entrainment rate varies with

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{schematic_diagram.png}
\caption{Schematic diagram of a single impinging jet [8]}
\end{figure}
many parameters, including heat release, buoyancy, speed of the co-flow jet, and the axial
distance from the jet nozzle. The heat release effects are relevant in the current studies
and they are discussed here. The entrainment rates are lower in the reacting cases as the
entrained mass has lower density than that in the non reacting case. Han and Mungal
[38] showed that the heat release reduces the entrainment in the near field of reacting jets
by a factor of 2.5, which is close to \((T_b/T_u)^{0.5}\), where \(T_b\) and \(T_u\) are the burnt gas and
unburnt gas temperature respectively. These observations are based on the work done by
Hasselbrink [39], which showed that the flow speed is amplified by the same factor of 2.5
in the reacting case. This factor is close to \((\rho_u/\rho_b)^{0.5}\), which can be approximated by
\((T_b/T_u)^{0.5}\) in a constant pressure system. Here \(\rho_u\) is the unburnt gas density and \(\rho_b\) is the
burnt gas density. Since mass flux is defined by \(\dot{m}/A = \rho u\) and density decreases by a factor
of \((T_u/T_u)\), the entrainment rate reduces by a factor of \((T_b/T_u)^{0.5}\).

The entrainment effects, which are crucial in the efficient operation of the high temper-
ature air combustion are dealt in the literature [124]. A new entrainment rate called flame
entrainment is defined along the flame. The study analyzed the influence of heat release,
-oxygen concentration, fuel flow rate and preheat temperature. The conclusions are that (1)
the heat release decreases the entrainment and more uniform the heat release, the greater is
the entrainment, (2) the entrainment increases with decrease in the oxygen concentration,
and (3) the entrainment is independent of the fuel flow rate and the preheat temperature.

### 2.2 Turbulence Combustion Interactions

In most practical combustors, combustion occurs in the presence of turbulent flow. For
example, the mixing of fuel and air in the non-premixed combustion occurs in highly tur-
bulent zones. In fact, the jets that are injected into the combustor are usually highly
turbulent. The strong nonlinear interactions between turbulence and chemistry make tur-
bulent combustion harder to understand. Turbulence/chemistry interactions (TCI) have
been a central subject in the research of turbulent reacting flows. TCI arise from the fact
that mixing processes in turbulent flow are not fast compared with the rates of chemical
reactions. The time scales of chemical reactions can range from \(10^{-10}\) s to more than 1 s
The effect of turbulence on chemical reactions takes place through the large-scale stirring motions of turbulence. By stretching and curvature, the large-scale motions of turbulence enhance greatly the molecular diffusion rates of chemical species and heat, and therefore enhance greatly chemical reactions, which occur at molecular scales and must be balanced by molecular diffusion. The differential diffusion of chemical species also can become important. In addition, the turbulent motions produce large variations in species composition and temperature, which cause the mean reaction rates to be strongly coupled to molecular diffusion at the smallest scales of the turbulence. The effect of chemical reaction on turbulence takes place through the large heat release from chemical reactions. On one hand, the large heat release results in large density gradients, that produce a source term in the vorticity transport equation and therefore enhance the intensity of turbulence. On the other hand, the heat release produces local dilatation, which acts as a sink term in the vorticity equation and therefore reduces the intensity of turbulence. Furthermore, the heat release produces high temperature regions and therefore high viscosity regions, which enhance the diffusion of the vorticity in the turbulent flow field. The net effect of heat release on the turbulent intensity depends on the specific conditions in which chemical reactions occur in turbulent flows.

### 2.2.1 Combustion regimes

#### 2.2.1.1 Premixed combustion

Due to the presence of multitude of characteristic length and time scales in turbulent combustion, analyzing the phenomenon is an ardent task. Hence, using some non-dimensional numbers based on the characteristic scales, different combustion regimes are established in the literature [13, 82]. The main objective of this classification is to derive and choose turbulent combustion models. Since, many assumptions are involved in developing such a regime diagram, the analysis will be only qualitative. In the following discussion, all the scales and the non-dimensional numbers used in the regime diagram will be first defined and then discuss different regimes.
The regime diagram as proposed by Peters [81] is shown in Figure 4. It is mainly a $v'/S_L$ vs. $l/l_F$ plot, where $v'$ is the turbulent intensity, $S_L$ is the laminar flame speed, $l$ is the integral length scale of the turbulence and $l_F$ is the laminar flame thickness. $l_F$ is defined as $D/S_L$ (assuming equal diffusivities), where $D$ is the mass diffusivity. The other parameters that appear in Fig. 4 are $\eta$ (Kolmogorov scale) and $l_\delta$ is the inner layer, where $\delta$ represents the ratio of inner layer to flame thickness ($l_\delta/l_F$). The non-dimensional parameters that are used to mark the regimes are turbulent Reynolds number ($Re = v'l/S_L l_F$), Karlovitz number based on flame thickness ($Ka = l_F^2/\eta^2$) and Karlovitz number based on inner layer ($Ka_\delta = l_\delta^2/\eta^2$).

Following the above definitions, turbulent premixed flame regimes are proposed as:

- **Flamelet regime** ($Ka < 1$): This region is further divided into 2 zones.

  1. **Wrinkled flamelets** ($v'/S_L < 1$). In this regime the laminar flame speed is higher than the turbulent intensity. Hence the combustion phenomenon is mainly dominated by the chemistry and turbulence which only wrinkles the flame surface. Hence the TCI’s are limited in this regime.

  2. **Corrugated flamelets** ($v'/S_L > 1$). In this regime, flame structure is embedded
entirely inside the Kolmogorov eddies. Hence the flame structure is still not perturbed by turbulent fluctuations. Peters [82] suggest that there is kinematic interaction between the turbulent eddies and the laminar flame.

- **Thin reaction zone** ($Ka > 1$ and $Ka < 1$). Typically $\delta$ is taken as 0.1 and hence the corresponding $Ka = 100$. Thus thin reaction zones exist in the regions where karlovitz numbers lie between 1 and 100. In this regime, the small eddies can penetrate into the flame as $l_F < \eta$. However, the eddies can not penetrate into the inner as they are still larger than the inner layer. They can only enter the preheat zone and cause TCI’s. The flame still retains laminar like structure.

- **Broken reaction zone** ($Ka > 1$). In this zone, eddies can penetrate into both the preheat and the inner layers of the flame. Due to this, TCI’s are very predominant in this region. Laminar flame like structure can not identified in this zone. This region is of interest in flame stabilization studies as the effects of turbulence can cause local flame extinction that may lead to flame quenching.

Most of the practical applications fall under the corrugated flamelets or the thin reaction zones. Hence, most of the turbulence chemistry models are developed for this region. However, in a combustor, all the regions can simultaneously present at different locations and an ideal model should be the one that has applicability in all the regimes.

Pitsch [84] modified the above regime diagram for LES applications. LES based parameters are used to construct the regime diagram. The sub-grid velocity fluctuation $v'_\Delta$ is used instead of turbulent intensity $v'$ and the LES filter $\Delta$ are used instead of integral length scale $l$. Based on this, the subgrid Reynolds number $Re_\Delta$ is defined as $Re_\Delta = \frac{v'_\Delta}{\bar{\nu}}$. The definitions of Karlovitz numbers will still be same as before. Figure 5 shows the Regime diagram using the modified definitions. The Figure still shows the similar classification of zones as proposed by Peters [82].
2.2.2 Non-premixed combustion

There are no established regime diagram for non-premixed combustion. The problem is that the diffusion do not propagate, and therefore there is no characteristic speed scale. Also, the flame thickness is determined by the local mixing between fuel and air. Hence, identification of a fixed length and speed scale can not be easily identified in the diffusion flames.

A regime diagram for the non-premixed turbulent combustion is given by Veynante [85] based on the Damkohler number $Da$ (ratio of integral time scale and chemical time) and the turbulent Reynolds number. A schematic sketch of the regimes is shown in Figure 6. The diagram shows the the laminar flamelet assumption (LFA) validity regions, the quenching limits and the zones where unsteady and curvature effects are important. The two limiting Damkohler number $Da_{LFA}$ and $Da_{ext}$ separate these regimes. Like in the premixed case, practical non-premixed combustor can operate in different regimes at different locations.

2.2.3 Modeling

With the recent advances in computer technology, the Computational Fluid Dynamics (CFD) is fast becoming more and more feasible. Simulations are being used to tackle
the problem of turbulent combustion. However, the modeling is not straightforward due to incomplete understanding of the phenomenon. Basically, the turbulent combustion modeling can be divided into three sub-problems.

- Turbulence modeling, which by itself is a very complex phenomena.

- The specific combustion model without turbulence, which is also a quite complex process involving many chemical reactions in very short times. There are models ranging from the simpler no-model Arrhenius approach to more complex ones like laminar flamelets models [80]

- The modeling of the interaction between combustion and a turbulent flow. From the above discussion on TCI, this one can be divided into two set of problems: the effects of turbulence on the flame front (often taken into account by the more complex combustion models), and the problem of flame generated turbulence.

Thorough details of all the above processes are not presented here. However, some details, in particular from the modeling frame work, that are in the scope of this work are presented here.
2.2.3.1 Turbulence modeling

The modeling of turbulent flow remains one of the great scientific challenges. It is well known that large range of length scales (corresponding time and velocity scales) are present in turbulent flows and that kinetic energy is transferred from larger scales to smaller scales, where viscous effects convert the kinetic energy to thermal energy. This is the so called energy cascade and the smallest scale in this cascade that can transfer energy is the Kolmogorov scale ($\eta$). The dynamics of the turbulence is governed by these range of scales. Hence, accuracy of the numerical simulations depend on the resolution of of these scales. Based on the range of scales that are resolved in a flow, numerical methods are classified into 3 main categories [89].

- **Direct Numerical Simulations (DNS):** In these simulations, all the scales are resolved to characterize turbulence. However, the range of scales depend on the Reynolds number (ratio of inertial forces/viscous forces) of the flow and grid requirement scales as $Re^{9/4}$. Hence, to simulate a flow with $Re = 10^4$, number of grid points required is $10^9$. In addition, the flow must evolve in time which requires tremendous computational resources (note that this is without combustion). Despite the dramatic advances in computing power over the last decade, a complete unsteady DNS study of practical combustor flows (where $Re$ can be in excess of 10,000) remains out of question.

- **Large Eddy Simulations (LES):** In LES, large scales are resolved while the small scale effects are modeled. Usually, large scales that contain most of the energy are associated with the geometry and hence will differ for different flows. However, as the scales get smaller and smaller, they will loose the geometry information and hence can be more universal. This was stated by Kolmogorov in his first hypothesis as "In every turbulent flow at sufficiently high Reynolds numbers, the statistics of the small scale motions have a universal form that is uniquely determined by kinematic viscosity ($\nu$) and dissipation rate ($\epsilon$)". Hence, a small scale model that has generic applicability can be found, while the large scales need to be resolved. This is the main postulate of LES technique.
Reynolds Averaged Navier Stokes (RANS) approach: In this approach, none of the scales are resolved. All the turbulent scales are modeled as an single scale. RANS solves for the time averaged quantities.

The main advantage of RANS is that, it is the least expensive among the three approaches. Hence, it is a favored tool in engineering applications. However, the main disadvantage is that only mean field is provided by the simulation. RANS calculation can not provide the information about the vortex dynamics, which is crucial in the prediction of turbulent chemistry interactions [83]. In addition, models are required to close the terms that result from time averaging of Navier Stokes equations. DNS is currently restricted to pursue academic studies. LES is only approach that is both accurate and computationally feasible. LES is widely considered [83] to be a promising approach for combustion studies. Since LES solves the unsteady and intermittent behaviour of the large scale eddies that are responsible for mixing [74]. The accuracy of the combustion models depend on the accuracy of the the fluid dynamics. Hence, LES can provide far more accurate description then RANS. It is also established as a powerful tool to predict the occurrence of combustion instabilities, which when present can damage the entire system. LES also can provide better description of TCI’s between the resolved flow scales and the chemical scales.

In spite of many advantages, combustion LES poses modeling issues. LES also needs models to close the terms that result from filtering of the Navier Stokes equations. A sub-grid model is still needed to represent the small scale effects. Now, it is well known that combustion occurs at molecular scales i.e. scales at which the dissipative effects are dominant. Hence, combustion occurs at scales below the grid size and hence must be modeled. Thus, in reacting cases, the sub-grid models need to predict both the sub-grid momentum transport and sub-grid combustion. And the interaction of the sub-grid eddies with the chemical scales must also be properly represented. Thus, a sub-grid model must be able to represent the multi-scale phenomena in turbulent combustion, and must accurately represent the interaction between resolved and unresolved scales. The model must also must account for the the sub-grid processes; molecular diffusion and chemical reactions. To carry out these aspects of turbulent combustion, a number of models are established in the
literature. A brief review of these models is provided below.

2.2.4 Turbulence chemistry closures

As mentioned previously, the turbulence chemistry model plays the most important role in the accurate prediction of turbulent combustion. The choice of the model forms the crux of most of the numerical studies on practical combustor studies. This subsection is aimed at reviewing some of the established models in the literature. Some of these models are applicable in specific regimes or specific combustion modes. Some others more general.

2.2.4.1 The Eddy Break Up model (EBU)

This model was first developed by Spalding [109] and extended to LES applications by Fureby and Lofstrom [32]. It is based on the assumption that chemistry time is much faster than the mixing time and thus, the rate controlling mechanism is the turbulent mixing. Such an assumption will predict very high reaction rates in the shear layers where turbulence levels are very high. Hence, a variant of this model (sometimes referred to as eddy dissipation model) is proposed where the reaction rate is computed as the minimum of the kinetic reaction rate and the mixing rate. The most severe draw back of this approach is the use of ad hoc model constants. The model is very simple and is very easy to implement. This simple description of the chemical reaction in turbulent flows is too simple to yield any accurate prediction of the TCI’s. The main advantage is that the procedure is computationally inexpensive. This model can be implemented in both premixed and non-premixed modes. However, it only serve as a preliminary study.

2.2.4.2 Artificial Thickened Flames (TF)

This approach is applicable in premixed flame applications. In typical premixed flames, the flame front is very thin and it must be resolved to capture the inner structure. This is not possible on typical LES meshes. An approach to overcome is to artificially thicken the flame so that it can be resolved on the LES mesh. However, the flame should be propagating at the same speed as the unthickened flame. This is achieved following simple theories of laminar premixed flames. The laminar flame speed $S_L$ and the laminar flame thickness $l_F$
may be expressed as:

\[ S_L \propto \sqrt{DW}, \quad l_F \propto D/S_L \]  

(4)

where \( D \) is the molecular diffusivity and \( \overline{W} \) is the mean reaction rate. Then an increase in flame thickness by factor \( F \) with a constant flame speed can be obtained by multiplying mass diffusivities \( D \) by \( F \) (the same should be done with thermal diffusivity also) and by replacing reaction rate \( \overline{W} \) by \( \overline{W}/F \). This is the basic principle of TF. Colin et al. [21].

TF is very well established in the literature for premixed flames and is shown to predict ignition, quenching, blow-off [108], and combustion instabilities [3]. These are some drawbacks also. By artificially thickening the flame, the effects of the turbulent eddies on the flame are missing in the model. Hence, the sub-grid scale effects are incorporated into the model using an efficiency function (\( E \)) derived from DNS results. The generic applicability of these efficiency functions is yet to be explored. Furthermore, the model cannot handle the complex chemical mechanisms. As of now, either single or 2 step mechanisms are used with this model. This is because the approach becomes questionable once intermediate steps are involved. In particular, a highly diffusive species like \( H \) can impose prohibitive thick flames inside the combustor.

2.2.4.3 Laminar Flamelets

Laminar Flamelet assumptions are valid in the region where the chemical scales are faster than the mixing and that the flame structure resembles a laminar-like structure. In these regimes, a turbulent flame can be assumed as consisting of an ensemble of stretched laminar diffusion flames [122]. This approach led to a family of modeling approaches to model the premixed and the non-premixed combustion. Typically, in these models, the flame surface is tracked using an iso-surface of a non-reacting scalar. These scalars are usually denoted as \( G \) in premixed mode and \( Z \) in non-premixed mode or some kind of progress variable. Once these scalars are evaluated in the flow, flamelet libraries are used to obtain the species (reactive scalars).
2.2.4.4 The Probability Density Function (PDF) models

In PDF methods [87], the chemical state of the reacting mixture is defined by the joint PDF of velocity and reactive scalars and/or joint PDF of reactive scalars and temperature and species or other quantities of interest. So, these models either predict the shape or form of PDF or solve them by evolving their transport equations. Once, the PDF is known, the reaction rates can be computed without any closure issues. This is the main advantage of the PDF models. The reaction rate requires no closure. However, the diffusion terms in the PDF equations needs modeling, which is a limitation of the model. Since no prior information of the flame is needed, these models are applicable in all the combustion regimes and in both the premixed and non-premixed modes.

Depending on the approaches used to describe PDF, the models can be classified into 2 categories

- **Presumed PDF methods** In these methods, PDF is assumed based on the observations in experiments. Hence, the inaccuracies in these models will be mainly to the choice of the distributions. In most of the studies, the presumed PDF follow an analytical distribution such as a $\beta$ function.

- **Transported PDF models** In this category, an exact transport equation of the PDF is solved. Due to their generic applicability, these models are gaining importance. However, a mixing model needs to be implemented in PDF methods. This remains a main drawback as in molecular mixing controls chemical reaction and heat release. Moreover, these simulations are computational very expensive. These models give rise to numerical oscillations in density values. Generally, the flow variables are solved using finite volume approach whereas the PDF transport equations are solved using Monte-Carlo methods. Due to this inconsistency, numerical noise is reported in density calculations, which forms the main link between the hydrodynamic solver and the particle solver [42].
2.2.4.5 The Linear Eddy Mixing (LEM) model

The development of LEM is motivated by the understanding of the turbulent combustion phenomenon. The basic idea is to develop a model that accurately represents the turbulent combustion. The LEM model discriminates the different characteristic scales in the flow and resolves the physical processes such as advection, turbulent mixing, molecular mixing, and chemical reaction. It was originally formulated for non-reacting flows [44, 46, 47] and later extended to reacting flows [49, 48, 50]. LEM was first used as sub-grid model by Menon et al. [69]. This approach, referred to as LEMLES hereafter, has been developed to offer a closure directly at the sub-grid scales for all combustion processes. The scalar evolution in LEMLES is solved by simulating molecular mixing and chemical reaction in a one-dimensional domain embedded in a turbulent flow. This is followed by a stochastic rearrangement events called triplet mapping [45] to represent the action of an individual eddy on the scalar field. LEMLES approach is extensively used in this work and hence more details are provided later.

The only requirement for this mixing model is the Reynolds number independence of free shear flows in the limit of large Reynolds numbers, which is a safe assumption for any flow of engineering interest [82]. Due to this independence on the flow parameters other than Reynolds number, the LEM model can be expected to perform well in any combustion regime [66], irrespective of the combustion mode and can accurately handle flames near to, or even outside, the flammability limits [26]. LEMLES had been successfully applied to scalar mixing [18, 99], premixed combustion [17, 100, 26], non-premixed combustion [68, 15], pollutant emission [26], spray combustion [70] and sooting flames [28] without requiring ad hoc model changes. Since the processes on 1D line are resolved up to the smallest scales, this approach can be relatively expensive than the other closure models (except transport PDF methods). However, the computational time can be greatly reduced by performing simulations in a parallel environment. In the current implementation, laminar diffusion across LES cells is not implemented. Since LEMLES is designed for high Reynolds number turbulent flow applications, this might not be a disadvantage. Also, the viscous work is neglected in the sub-grid temperature equation, but it is explicitly included in the
LES energy equation. Note that even though the sub-grid temperature is evolved within LEM, the LEMLES approach computes the resolved temperature based on total energy conservation equation in LES. More details are provided in chapter 3. Finally, the flame front curvature effects are not explicitly accounted at the sub-grid level. The curvature effects play a role in the flame turbulence interactions if the flame is highly wrinkled with multiple flames in the sub-grid LEM domain. This kind of situation can occur if the LES grid is coarse in the regions of high turbulence [90]. Hence, for the cases simulated in this study, the LES grid resolution is chosen to resolve the turbulence in the shear layers where the flame wrinkling effects are predominant.

The current studies employ the EBULES, TFLES and LEMLES approaches in the reacting simulations. The mathematical description and their numerical implementation are provided in the later chapters.
CHAPTER III

MATHEMATICAL FORMULATION AND MODELING

This chapter provides details of the relevant equations and the models used in this study. The first section provides the governing equations and the second section deals with the turbulence-chemistry closures which forms the crux of this study.

3.1 Governing Equations

The governing equations of motion for an unsteady, compressible, reacting, multiple-species fluid are the Navier-Stokes equations. Using these equations, the filtered equations for the LES are obtained. The following subsections provide details of these equations.

3.1.1 The Navier-Stokes equations

The Navier-Stokes equations are the exact form of the governing equations in the absence of the dispersed phase source terms and are written as:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0 \\
\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho u_i u_j + p \delta_{ij} - \tau_{ij} \right] &= 0 \\
\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i} \left[ \rho E + p \right] u_i + q_i - u_j \tau_{ij} &= 0 \\
\frac{\partial Y_m}{\partial t} + \frac{\partial}{\partial x_i} \left[ \rho Y_m (u_i + V_{i,m}) \right] &= \dot{w}_m \text{, where } m = 1, N
\end{align*}
\]

In the above equations, \( \rho \) is the mass density, \( u_i \ (i = 1, 2, 3) \) are the velocity components, \( p \) is the pressure, \( \delta_{ij} \) is the Kronecker function \( (\delta_{ij} = 0 \text{ if } i \neq j \text{ and } \delta_{ij} = 1 \text{ if } i=j) \) and \( \tau_{ij} \) is the viscous stress tensor, defined as:

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

where \( \mu \) is the molecular viscosity coefficient. Also, in equation 5 \( E \) is the total energy per unit mass given by \( E = e + \frac{1}{2} (u_k u_k) \), where \( e \) is internal energy per unit mass computed as:

\[
e = \sum_{m=1}^{N} Y_m h_m - \frac{p}{\rho}
\]
where \( h_m \) is the species enthalpy per unit mass given by:

\[
h_m(T) = \Delta h_{f,m}^0 + \int_{T_0}^{T} c_{P,m}(T')dT'
\]  

(8)

In the above equation, \( \Delta h_{f,m}^0 \) is the enthalpy of formation per unit mass of the \( m \)-th species at the reference temperature \( T_0 \), \( c_{P,m} \) is the specific heat at constant pressure for the \( m \)-th species.

Again, referring to equation 5, \( q_i \) is the heat flux in \( i \)-th direction, \( Y_m \) is the \( m \)-th species mass fraction and \( V_{i,m} \) is the diffusion velocity of the \( m \)-th species in the \( i \)-th direction and \( \dot{\omega}_m \) is the mass reaction rate per unit volume of the \( m \)-th species.

The heat flux vector \( q_i \) contains the thermal conduction (I), enthalpy diffusion (i.e. diffusion of heat due to species diffusion) (II), the Dufour heat flux, and the radiation heat flux. Dufour heat flux and radiation heat flux are neglected here, therefore:

\[
q_i = -\kappa \frac{\partial T}{\partial x_i} + \rho \sum_{m=1}^{N} h_m Y_m V_{i,m}
\]  

(9)

where \( \kappa = \tau P_P/Pr \) is the mixture averaged thermal conductivity. \( \tau P = \sum_{m=1}^{N} Y_m c_{P,m} \) is the mixture averaged specific heat at constant pressure and \( Pr \) is the mixture Prandtl number.

The diffusion velocities are approximated by Fickian diffusion as,

\[
V_{i,m} = -\frac{D_m}{\sum_{m=1}^{N} Y_m} \frac{\partial Y_m}{\partial x_i}
\]  

(10)

where \( D_m \) is the mixture averaged molecular diffusion coefficient. Diffusion due to the gradients of temperature (Soret) and pressure (Dufor) are neglected and no body forces are also included.

The mass reaction rate is:

\[
\dot{\omega}_m = MW_m \sum_{k=1}^{L} \left( \nu''_{mk} - \nu'_{mk} \right) A_k T^{\alpha_k} e^{(-E_{a,k}/RT)} \prod_{n=1}^{N} \left( \frac{X_{m,n}}{R_u T} \right)^{\nu'_n} \]  

(11)

where \( L \) is the number of chemical reactions of the considered chemical mechanism, \( N \) is the number of species, \( MW_m \) is the mass fraction of the \( m \)-th species, \( \nu''_{mk} \) and \( \nu'_{mk} \) are the stoichiometric coefficients of the \( m \)-th species and for the \( k \)-th chemical reaction on
the product and reactant side, respectively. $A_k$, $\alpha_k$ and $E_{a,k}$ are the Arrhenius rate pre-exponential coefficient, temperature exponent and activation energy for the $k$-th chemical reaction, respectively, $T$ is the temperature and $R_u$ is the universal gas constant. $X_m$ is the molar fraction of the $m$-th species.

The pressure $p$ is derived from the equation of state for perfect gas:

$$p = \rho RT = \rho \frac{R_u}{MW_{mix}} T = \rho R_u T \sum_{m=1}^{N} \frac{Y_m}{MW_m}$$  \hspace{1cm} (12)

The molecular viscosity is determined using Sutherland’s law:

$$\frac{\mu}{\mu^0} = \left(\frac{T}{T_0}\right)^{3/2} \left(\frac{T}{TS}\right)^{3/4}$$  \hspace{1cm} (13)

where $\mu^0$ is the reference viscosity at $T^0$ and $TS = 110.4$ K.

Finally, total mass conservation is enforced by constraining the species mass fractions and diffusion velocities using the following identities:

$$\sum_{m=1}^{N} Y_m = 1$$  \hspace{1cm} (14)

$$\sum_{m=1}^{N} V_{im} = 0, \ i = 1, 2, 3$$  \hspace{1cm} (15)

### 3.1.2 LES Mathematical Model

The mathematical model is the set of LES equations [65] which are derived from the Navier-Stokes equations given in equation 5 by an averaging procedure. The procedure involves filtering out the chaotic, fluctuating small scale high frequency motions and modeling their effect on the slowly varying smooth large eddies. The separation between the large and the small scales is determined by the grid size ($\Delta$). Therefore, the Navier-Stokes equations are filtered with respect to the grid size in order to obtain the LES governing equations.

The flow variables are decomposed into the resolved and unresolved (sub-grid) components by using a filtering operation such as $f = \bar{f} + f''$, where tilde “$\bar{f}$” denotes resolved scale and double prime “$''$” denotes unresolved sub-grid scale quantities. The $\bar{f}$ is the Favre filtered
Stokes equations can be written as \[29\]:
\[
T
ature
variable
and
is
defined
as
\(\tilde{f} = \bar{\rho} \bar{f} / \bar{\rho} \)
where
the
overbar
represents
the
spatial
filtering
\[29\]
and
is
defined
as
\[
\tilde{f}(\bar{x}, t) = \int_D f(x', t)G_f(\bar{x}, \bar{x}')dx'
\]
where
\(D\)
is
the
entire
computational
domain,
\(\bar{x}\)
is
the
position
vector
and
\(G_f\)
is
the
top-hat
filter
kernel
defined
as:
\[
G_f(\bar{x}, \bar{x}') = \begin{cases} 
\frac{1}{\pi} & \text{if } |\bar{x} - \bar{x}'| < \frac{1}{2} \\
0 & \text{otherwise}
\end{cases}
\]
By
applying
the
above
described
filtering
process
to
Eq.
5,
the
LES
filtered
Navier-
Stokes
equations
can
be
written
as
\[29\]:
\[\begin{align*}
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} &= 0 \\
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} &= 0 \\
\frac{\partial \bar{\rho} \bar{E}}{\partial t} + \frac{\partial \bar{\rho} \bar{H}_k}{\partial x_k} &= 0 \\
\frac{\partial \bar{\rho} \bar{Y}_k}{\partial t} + \frac{\partial \bar{\rho} \bar{W}_i}{\partial x_i} &= \tilde{w}_k
\end{align*}\]
where
all
terms
with
superscript
\textit{sgs}
denote
sub-grid
quantities
that
require
closure.
Also
\(\tilde{\tau}_{ij}\)
is
the
filtered
viscous
tensor,
and
\(\tilde{q}_i\)
is
the
filter
heat
flux
vector
given
by:
\(\tilde{q}_i = -k \frac{\partial \bar{f}}{\partial x_i} + \bar{\rho} \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} + \frac{\sum_{k=1}^{N_s} \bar{h}_k \bar{V}_{i,k} + \sum_{k=1}^{N_s} \bar{q}_{i,k}}{\sum_{k=1}^{N_s} \bar{q}_{i,k}}\). The filtered diffusion
velocities
are
approximated
using
Fickian
diffusion
as
\(\bar{V}_{i,k} = (-\bar{D}_k / \bar{Y}_k)(\partial \bar{Y}_k / \partial x_i)\).
The
pressure
is
determined
from
the
filtered
equation
of
state,
\(\bar{p} = \bar{\rho} \bar{R} \bar{T} + T^{\text{sgs}}\).
Here,
\(T^{\text{sgs}}\)
is
the
temperature-species
correlation
term
defined
as
\((\bar{Y}_k T - \bar{Y}_k \bar{T}) / W_m\).
The
filtered
total
energy
per
unit
volume
is
given
by:
\[\bar{p} \bar{E} = \bar{\rho} \bar{e} + \frac{1}{2} \bar{\rho} \bar{u}_i \bar{u}_i + \bar{\rho} k^{\text{sgs}}\]
where
the
sub-grid
kinetic
energy
is
defined
as,
\(k^{\text{sgs}} = (1/2)[u_k \bar{u}_k - \bar{u}_k \bar{u}_k]\).
The
filtered
internal
energy
for
calorically
perfect
gases
is
given
by
\(\bar{e} = \sum_{k=1}^{N_s} [c_{v,k} \bar{Y}_k \bar{T} + \bar{Y}_k \Delta h'_{f,k}]\) where,
\(\Delta h'_{f,k} = \Delta h^0_{f,k} - c_{p,k} T^0\),
and
\(\Delta h^0_{f,k}\)
is
the
standard
heat
of
formation
at
a
reference
temper-
ature
\(T^0\).
The
sub-grid
terms
that
require
closure
are:
\[\tilde{\tau}_{ij}^{\text{sgs}} = \bar{p} (\bar{u}_i \bar{u}_j - \bar{u}_j \bar{u}_i)\]
\[H^{\text{sgs}}_i = \bar{p} (\bar{E} \bar{u}_i - \bar{\rho} \bar{u}_i) + (\bar{W}_i - \bar{\rho} \bar{u}_i)\]
\[ \sigma^{sgs}_{ij} = u_j \tau_{ij} - u_i \tau_{ij} \]
\[ T^{sgs} = (Y_k T - \tilde{Y}_k \tilde{T})/W_m \]
\[ Y_{i,k}^{sgs} = \bar{\rho} [u_i \tilde{Y}_k - \bar{u}_i \tilde{Y}_k] \]
\[ q_{i,k}^{sgs} = \left[ h_k D_k \partial Y_k / \partial x_i - \tilde{h}_k \tilde{D}_k \partial \tilde{Y}_k / \partial x_i \right] \]
\[ \theta_{i,k}^{sgs} = \bar{\rho} [V_{i,k} \tilde{Y}_k - \bar{V}_{i,k} \tilde{Y}_k] \] (22)

Here \( \tau_{ij}^{sgs} \) is sub-grid shear stress, \( H_i^{sgs} \) is sub-grid enthalpy flux, \( \sigma_i^{sgs} \) is sub-grid viscous work, \( Y_{i,k}^{sgs} \) is convective species flux, \( q_{i,k}^{sgs} \) is sub-grid heat flux and \( \theta_{i,k}^{sgs} \) is sub-grid species diffusive flux.

3.1.3 SGS Closure for LES equations

Many approaches have been proposed by the research community to close the sub-grid terms in LES. Model for sub-grid stress tensor \( \tau_{ij}^{sgs} \) is usually derived by using an analogy between the viscous stresses \( \tau_{i,j} \) in the unfiltered Navier-Stokes equations and the sub-grid stresses in the filtered equations. Using the analogy, the sub-grid stress tensor \( \tau_{ij}^{sgs} \) is modeled as:
\[ \tau_{ij}^{sgs} = -2 \rho \nu_t [S_{ij} - \frac{1}{3} S_{kk} \delta_{ij}] + \frac{3}{2} \beta k^{sgs} \delta_{ij}. \]
To complete the closure for the sub-grid stresses, the sub-grid eddy viscosity, \( \nu_t \) and the sub-grid kinetic energy, \( k^{sgs} \) need to be modeled. The simplest is the algebraic eddy viscosity model proposed by Smagorinsky [104], which is based on the assumption that sub-grid kinetic energy production and dissipation balance each other. This requirement is satisfied only in the dissipation range of turbulent spectrum. Most of the engineering applications involve high Reynolds numbers. The LES grid resolution will not be sufficient to resolve the dissipation range. Thus, the equilibrium requirement is not met in these cases. Hence, a non-equilibrium model using a transport equation for the sub-grid kinetic energy, \( k^{sgs} \) was developed by Schumann [101]. The current study will follow the implementation given by Menon et al. [71], where a transport equation was formally derived for \( k^{sgs} \) and solved along with the rest of the LES equations. Since \( k^{sgs} \) evolves locally and temporally in the flow, the equilibrium assumption is relaxed. Hence, the grid resolution needs to resolve scales up to the inertial range instead of the dissipation
range. The evolution equation is given by:

\[
\frac{\partial k_{sgs}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho}u_i k_{sgs}) = \frac{\partial}{\partial x_i} \left( \frac{\nu_t}{\sigma_k} \frac{\partial k_{sgs}}{\partial x_i} \right) + P_{sgs} - \epsilon_{sgs}
\]

The terms, \( P_{sgs} \) and \( \epsilon_{sgs} \) in the above equation are respectively, the production and the dissipation of sub-grid kinetic energy. The sub-grid dissipation, \( \epsilon_{sgs} = C_\epsilon \rho (k_{sgs})^{3/2} / \Delta \) where, \( C_\epsilon \) is a model coefficient. The sub-grid production term is modeled as \( P_{sgs} = -\tau_{ij} (\partial u_i / \partial x_j) \), and the the sub-grid eddy viscosity is modeled as \( \nu_t = C_\nu \sqrt{k_{sgs}} \Delta \), where \( C_\nu = 0.067 \) is another model constant. The coefficients \( C_\epsilon \) and \( C_\nu \) are evaluated using a localized dynamic procedure, the details of which are provided in the next subsection.

The sub-grid total enthalpy flux \( H_{i}^{sgs} \) is modeled using the eddy viscosity model as follows:

\[
H_{i}^{sgs} = (-\bar{\rho} \nu_t / Pr_t) (\partial \bar{H} / \partial x_i),
\]

where \( Pr_t \) is the turbulent Prandtl number currently assumed to be unity. \( \bar{H} \) is the total enthalpy term and is evaluated as \( \bar{H} = \bar{h} + \bar{u} \bar{u} / 2 + k_{sgs} \), where \( \bar{h} = \sum_{k=1}^{N} \bar{h}_k \bar{Y}_k \). The sub-grid terms, \( \sigma_{i}^{sgs} \), \( \dot{q}_{i,k}^{sgs} \) and \( T^{sgs} \) are neglected here based on past studies [33].

3.1.4 Localized dynamic kinetic energy model (LDKM)

In the present study, \( C_\epsilon \) and \( C_\nu \) are dynamically computed as a part of the solution using the flow conditions. The approach was developed by Kim and Menon [51] for incompressible flows and was extended by Nelson and Menon [76] for compressible flows. The model is based on the assumption that there exists a scale similarity in the inertial sub-range turbulence. The basic premise of scale similarity is that the largest unresolved sub-grid scales are statistically similar to the smallest resolved scales. To obtain scale similar expressions, a test filter, denoted by \( \tilde{\cdot} \) is defined close to the cutoff scale (grid filter), but at the resolved scales. The size of the test-filter is twice the LES resolution: \( \tilde{\Delta} = 2\Delta \). Note that the grid-filter at the LES cut-off limit operates on the exact equations, whereas the test filter operates on the grid-filtered variables. Experimental studies [61] in high Reynolds number turbulent jet have shown that the sub-grid stress \( \tau_{ij}^{sgs} \) at the grid filter level and the Leonard’s stress \( L_{ij} \) \( \left( = \frac{\tilde{p} \tilde{u}_i \tilde{u}_j - \tilde{p} \tilde{u}_i \tilde{u}_j}{\tilde{p}} \right) \) at the test filter level are self-similar. A simple scale-similar model of the form \( \tau_{ij}^{sgs} = C_L L_{ij} \), where \( C_L \) is an adjustable constant [61] was found to lack turbulent dissipation. Hence, in LDKM, the above observation is extended.
and assumed the self-similarity between the Leonard’s stress at the test filter level and the sub-grid stress also at the test filter level. Therefore, \( \tau_{ij}^{s_{gs}} = \tilde{C}_L L_{ij} \) and Leonard’s stress can be written as:

\[
L_{ij} = \frac{\tau_{ij}^{s_{gs}}}{\tilde{C}_L} = -2\tilde{C}_L \sqrt{k_{test}} \Delta \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} \tilde{C}_L k_{test} \delta_{ij}
\]  

(23)

where \( k_{test} \) is the kinetic energy at the test filter level given by

\[
k_{test} = \frac{1}{2} \left( \frac{\tilde{p}_{uk}^2}{\tilde{\rho}} - \frac{\tilde{p}_{uk}^2}{\tilde{\rho}} \right)
\]

(24)

Evaluating \( s_{gs} \) at the test filter and equating to 23, will result in an over-determined system with 5 independent equation and one unknown \( C_L \). Assuming \( C_L = 1 \) and using least-square method [58], an expression of \( C_L \) is obtained.

\[
C_L = \frac{D_{ij} M_{ij}}{2 D_{ij} D_{ij}}
\]

(25)

where \( M_{ij} \) and \( D_{ij} \) are given below:

\[
M_{ij} = \tilde{\rho} \tilde{u}_j \tilde{u}_i - \frac{\tilde{\rho} \tilde{u}_j \tilde{u}_i}{\tilde{\rho}} - \frac{1}{3} \left( \tilde{\rho} \tilde{u}_k \tilde{u}_k - \frac{\tilde{\rho} \tilde{u}_k \tilde{u}_k}{\tilde{\rho}} \right) \delta_{ij}
\]

\[
D_{ij} = \Delta \tilde{\rho} \left( \frac{\tilde{u}_k \tilde{u}_k}{2 \tilde{\rho}} - \frac{\tilde{u}_k \tilde{u}_k}{2 \tilde{\rho}} \right) \frac{1}{2} \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right)
\]

(26)

\( C_\epsilon \) is obtained using similar approach [54, 52] and is given by:

\[
C_\epsilon = \frac{\Delta (\tilde{\rho} + \mu_t)}{\tilde{\rho} k_{test}^{3/2}} \left( \tilde{T}_{ij} \frac{\partial \tilde{u}_j}{\partial x_i} - \tilde{T}_{ij} \frac{\partial \tilde{u}_j}{\partial x_i} \right)
\]

(27)

where \( \mu \) is the molecular viscosity, \( \mu_t = \nu_t \tilde{\rho} \) is the eddy viscosity at the test level and the tensor \( \tilde{T}_{ij} \) is defined at the test filter level as:

\[
\tilde{T}_{ij} = \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij}
\]

(28)

The sub-grid stresses approach must satisfy realizability conditions. A realizable solution is obtained by imposing \( \tau_{ij}^{s_{gs}} \) to be positive and finite [75]. These constraints are summarized below [120]:
\[
\begin{align*}
\tau_{11}^{\text{sgs}} & \geq 0 \\
\tau_{22}^{\text{sgs}} & \geq 0 \\
\tau_{33}^{\text{sgs}} & \geq 0 \\
|\tau_{12}^{\text{sgs}}|^2 & \leq \tau_{11}^{\text{sgs}} \tau_{22}^{\text{sgs}} \\
|\tau_{13}^{\text{sgs}}|^2 & \leq \tau_{11}^{\text{sgs}} \tau_{33}^{\text{sgs}} \\
|\tau_{23}^{\text{sgs}}|^2 & \leq \tau_{22}^{\text{sgs}} \tau_{33}^{\text{sgs}} \\
\text{det}(\tau_{ij}^{\text{sgs}}) & \leq 0
\end{align*}
\]

The LDKM model as presented here was successfully used in many non-reacting [71, 79] and reacting [54, 53, 26, 70] studies. Its advantage is the local stability (in both space and time) without any smoothing procedures. This makes the model easy to implement in complex geometries. Past studies [31, 41], and the implementation of the model in commercial codes (Fluent v6.2.16 and higher) has demonstrated the reliability and accuracy of the LDKM closure. The model was found to be effective in the near wall region in turbulent wall bounded flows [31, 79].

### 3.2 Combustion Modeling

Several terms in Eqs. 17 still remain open at this point: the subgrid convective \( Y_{i,k}^{\text{sgs}} \) and diffusive \( \theta_{i,k}^{\text{sgs}} \) species fluxes, the subgrid heat flux, \( q_{i,k}^{\text{sgs}} \) and the filtered reaction rate, \( \overline{w}_k \) of the \( k \)th species. In this study, three approaches towards closing these terms are considered: two conventional closure at the LES resolved scales and a closure directly at the subgrid scales.

#### 3.2.1 Eddy Break - Up model (EBU)

The conventional closure for the species equations employs for the sub-grid convective scalar flux an eddy diffusivity closure as:

\[
Y_{i,k}^{\text{sgs}} = -\overline{\rho \nu_t} \frac{\partial \overline{Y}_k}{\partial x_i} \tag{30}
\]

where \( Sc_T \) is a turbulent Schmidt number that is set to unity in this study. Note that, \( \nu_t \) which is the turbulent diffusivity is obtained dynamically. There are no existing conventional
closure models [85] for the sub-grid heat flux, $q_{i,k}^{\text{sgs}}$, the sub-grid diffusive species flux, $\theta_{i,k}^{\text{sgs}}$, and the sub-grid temperature-species correlation, $T^{\text{sgs}}$. These terms are neglected here.

An approach based on a sub-grid EBU approach developed earlier by [32] is implemented to close the $\overline{\omega}_k$. The basic idea is that for combustion to occur, two processes need to take place simultaneously: chemical reaction and scalar mixing, and the rate controlling phenomena will be the slower of the two. The mathematical formulation of the model is provided below.

For a general reaction mechanism comprising of $N_r$ reactions given by $\sum_{k=1}^{N_s} \nu'_{k,j} M_{k,j} = \sum_{k=1}^{N_s} \nu''_{k,j} M_{k,j}$ the filtered reaction rates for species “$k$” is computed as follows $\overline{w}_k = W_k \sum_{j=1}^{N_r} (\nu''_{k,j} - \nu'_{k,j}) \min[q_{mix}^j, q_{kin}^j]$ where $q_{mix}^j$ and $q_{kin}^j$ are the molar reaction rates based on mixing and Arrhenius chemical kinetic rate, respectively. The Arrhenius reaction rates for step “$j$” is given by, $q_{j}^{\text{kin}} = k_{f,j} \prod_{k=1}^{N_s} [M_k]_{k,j}^{\nu''} - k_{b,j} \prod_{k=1}^{N_s} [M_k]_{k,j}^{\nu'}$ and the mixing rates for the forward and the backward reactions are given by

$$q_{j,f}^{\text{mix}} = \frac{1}{\tau_M} \min \left( \frac{[M_k]}{\nu'_{k,j}} \right) \quad \text{and} \quad q_{j,b}^{\text{mix}} = \frac{1}{\tau_M} \min \left( \frac{[M_k]}{\nu''_{k,j}} \right)$$

(31)

Here, $\tau_M$ is the mixing time scale and is related to the sub-grid turbulence as follows $\tau_M = C_{\text{EBU}} \frac{\overline{\omega}_k}{\sqrt{k_{\text{sgs}}}}$.

Although this approach (called EBULES hereafter) can provide reasonable results [33], it also has well known limitations. The most severe draw-back of this approach is the use of heuristic non-universal calibration constants. This description of the chemical reaction in turbulent flows is too simple to yield any reasonably good predictions, even though it is computationally cheap. Furthermore, the scalar fields at the sub-grid level are, unlike the turbulent scales, strongly anisotropic, thus rendering the use of the eddy diffusivity closure questionable.

### 3.2.2 Artificial thickened flame

The basic principle of this approach is to artificially thicken the flame so that it can be resolved on the LES mesh, but the flame should be propagating at the same speed as the unthickened flame. This is achieved by increasing the molecular diffusivities by a factor $F$ and decreasing the reactivities by the same factor. However, by thickening the flame,
the interaction between turbulence and chemistry is altered due to the reduction of the Damkohler number (flow time/chemical time). The action of the sub-grid scales on the flame front is missing in this approach. So, these effects are included using an efficiency function (E). The modifications are incorporated in the filtered species and energy equations. Thus, in TFLES, modeling is performed on both $Y_{i,k}^{sgs}$ and $\tilde{w}_k$ to account the sub-grid effects. The modified species and energy equations are solved along with the filtered mass and momentum equations. Only the modified filtered species equation is shown below.

$$\frac{\partial \tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} \left[ \tilde{p} \tilde{Y}_k \tilde{u}_i \right] - \tilde{p} E F \frac{\partial \tilde{Y}_k}{\partial x_i} + Y_{i,k}^{sgs} + \Theta_{i,k}^{sgs} = \frac{E \tilde{w}_k}{E \tilde{Y}_k}$$ (32)

Here $F$ and $E$ are the flame thickening factor and efficiency function, respectively. The sub-grid diffusive flux, $\Theta_{i,k}^{sgs}$ is neglected here, while the sub-grid convective flux $Y_{i,k}^{sgs}$ is closed using an eddy viscosity hypothesis as in equation 30. The value of $F$ is chosen to vary with the reaction rates. A maximum reaction rate based on the inflow conditions is computed everywhere along with the local reaction rate. Then $F$ is set to vary from a maximum value inside the flame to value of 1 far away from the flame.

$$\overline{S_{i_{max}}} = Y_{F_{max}} Y_{O_{max}}^2 e^{(-E_a/R 1600.0)}$$ (33)

$$\overline{S_i} = Y_F Y_O^2 e^{(-0.9E_a/RT)}$$ (34)

$$F = 1.0 + (FMAX - 1.0)tanh(S_i/S_{i_{max}})$$ (35)

Where $S_{i_{max}}$ and $S_i$ are the maximum and local rates, $Y_F$ and $Y_O$ are the fuel and oxidizer mass fractions, $E_a$ is the activation energy of the fuel break up step, $FMAX$ can be set to different values depending on the application. The expression for $F$ can give very high values because of which the maximum value of $F$ is restricted to 25 in the current studies.

The efficiency functions used in the current work are taken from Colin et.al. [21]. $E$ is expressed as a function of local filter size $\Delta_e$ (which is the grid size here), the laminar flame speed $s_L^0$, and the laminar flame thickness $\delta_L^0$ (unthickened flame) and $\delta_L^1$ (thickened flame).

$$E = \frac{\Xi(\delta_L^0)}{\Xi(\delta_L^1)} = (1 + \alpha \Gamma(\Delta_e, \frac{u'_{\Delta_e}}{s_L^0}) \frac{u'_{\Delta_e}}{s_L^0})(1 + \alpha \Gamma(\Delta_e, \frac{u'_{\Delta_e}}{s_L^0}) \frac{u'_{\Delta_e}}{s_L^0})^{-1}$$ (36)
where the function \( \Gamma \) accounts the effective strain rate induced by the scales in between kolmogorov and the gid size, \( \alpha \) is the model parameter that is a function of sub-grid Reynolds number. \( \Gamma \) is defined as:

\[
\Gamma\left(\frac{\Delta_e}{\delta_L}, \frac{u'_\Delta}{s_L^0}\right) = 0.75 \exp\left(-\frac{1.2}{(u'_\Delta/s_L^0)^{0.3}}\right)\left(\frac{\Delta_e}{\delta_L}\right)^{2/3}
\]

(37)

The sub-grid velocity is computed from the sub-grid turbulent kinetic energy assuming that all the sub-grid velocity components are same.

### 3.2.3 Linear-Eddy Mixing model

LEM is a stochastic approach aimed at simulating, rather than modeling the effects of turbulence on the chemistry. The only requirement for this mixing model is the Reynolds number independence of free shear flows in the limit of large Reynolds numbers, which is a safe assumption for any flow of engineering interest [82]. Due to this independence on the flow parameters other than Reynolds number, the LEM model can be expected to perform well in any combustion regime, irrespective of the combustion mode and can accurately handle flames near to, or even outside, the flammability limits.

In LEMLES, the species transport equations are not filtered, instead the large scale advection, molecular diffusion, turbulent mixing by eddies smaller than grid size, and chemical reaction are resolved at their respective time and length scales inside each LES cell. In order to describe this model mathematically, the velocity field is split as \( u_i = \bar{u}_i + (u'_i)^R + (u'_i)^s \).

Here, \( \bar{u}_i \) is the LES resolved velocity field, \( (u'_i)^R \) is the LES resolved sub-grid fluctuation (obtained from \( k^{sgs} \)), and \( (u'_i)^s \) is the unresolved sub-grid fluctuation. Now, consider a transport equation for a unfiltered reactive scalar \( Y_k \).

\[
\rho \frac{\partial Y_k}{\partial t} = -\rho\left[\bar{u}_i + (u_i')^R + (u_i')^s\right] \frac{\partial Y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho Y_k V_{i,k}\right) + \dot{w}_k
\]

(38)

In LEMLES, the above equation is rewritten as

\[
\frac{Y_k^{n+1} - Y_k^n}{\Delta t_{LES}} = -\left[\bar{u}_i + (u_i')^R\right] \frac{\partial Y_k^n}{\partial x_i}
\]

(39)

\[
Y_k^{n+1} - Y_k^n = \int_t^{t+\Delta t_{LES}} -\frac{1}{\rho} \left[\rho (u_i')^s \frac{\partial Y_k^n}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\rho Y_k V_{i,k}\right)^n + \dot{w}_k^n\right] dt'
\]

(40)
Here $\Delta t_{LES}$ is the LES time step. Equation (39) represents the transport of the scalar field by the resolved LES velocity field, and 40 represents small scale processes. The implementation of these equations is described below.

### 3.2.3.1 Small scale processes

Equation (40) describes the small scale processes as viewed at the LES space and timescales. The right hand side of the Eq. (40) represents three processes that occur within each LES grid: (1) sub-grid molecular diffusion, (2) chemical reaction, (3) sub-grid stirring. All these processes are modeled on a one-dimensional domain embedded inside each LES cell. The one-dimensional domain in each LES cell is not physically oriented along any of the Cartesian ($x,y,z$) directions, but oriented in the direction of the local, instantaneous maximum scalar gradient [45, 69]. The reaction-diffusion process is solved on the 1D domain using a grid that is resolved fine enough to resolve scales down to the Kolmogorov scale. As a result of this, the reaction-diffusion part of Eq. (40) is closed in an exact manner. The sub-grid stirring term is implemented using stochastic rearrangement events called triplet maps. Kerstein [45] demonstrated that triplet mapping is able to accurately capture the increase in the scalar gradient while maintaining the mean scalar field value. The mapping is performed using the isotropy assumption of the small scale eddies (subgrid velocity), which is consistent with the LES approach.

Mathematically, the triplet mapping transforms initial scalar field $\Psi^0(x,t)$ into a new scalar field, $\Psi(x,t)$:

\[
\Psi(x,t) = \begin{cases} 
\Psi^0(3x - 2x_0, t) & x_0 \leq x \leq x_0 + l/3 \\
\Psi^0(-3x - 2x_0 + 2l, t) & x_0 + l/3 \leq x \leq x_0 + 2l/3 \\
\Psi^0(3x - 2x_0 - 2l, t) & x_0 + 2l/3 \leq x \leq x_0 + l \\
\Psi^0(x, t) & \text{otherwise}
\end{cases} 
\]  

where $x_0$, $t_0$, and $l$ are the location, time, and eddy size of the mapping event respectively.

Thus, above three parameters are needed to perform turbulent stirrings. The eddy size $l$ which lies between $\Delta$ and $\eta$ is determined randomly from an eddy size distribution given
by Kerstein [45]:

\[ f(t) = \frac{(5/3)l^{-5/3}}{\eta^{-5/3} - \Delta^{-5/3}} \]  \hspace{1cm} (42)

where the Kolmogorov scale is determined as \( \eta = N_\eta \Delta Re \Delta^{4/3} \) and \( N_\eta \) is an empirical constant that reduces the effective range of scales between the integral length scale and \( \eta \) but without altering the turbulent diffusivity [107]. The value used for this study is 5 [107]. The event location is chosen from a uniform distribution and the event rate (mean frequency per unit length) is implemented as a Poisson process in time. This frequency is given by [45]:

\[ \lambda = \frac{54 \nu \Delta Re \Delta^3}{5 C_\lambda \Delta^3} \left[ \frac{(\Delta/\eta)^{5/3} - 1}{1 - (\eta/\Delta)^{4/3}} \right] \]  \hspace{1cm} (43)

where \( C_\lambda \) stands for the scalar turbulent diffusivity, set to 0.0675 [19].

3.2.3.2 Large scale processes

Equation 39 represents the large-scale advection of the scalar. This is modeled using an approach called Splicing, which involves lagrangian transport of the scalar field across LES cells and ensures exact mass conservation. After completing the sub-grid LEM processes in each LES cell, the sub-grid scalar fields are advected by the LES resolved velocity field. The method involves transfer of LEM cells between LES control volumes to account for the mass flux across the LES cell faces. To perform this, the magnitude of the mass flux that has to be transported and the direction of the mass flux on each cell face should be known. In a finite volume approach, both these quantities are known on each LES cell face. Now, the final advection operation must be performed in the 3-co-ordinate directions. This is numerically implemented by a sequence of three, one-dimensional advection operators. The order in which these three operations are performed is dictated by the magnitude of the mass flux in the respective direction at the resolved level. More details can be found elsewhere [68, 19, 106]. Now, for each LES cell, number of LEM cells that contains the mass that has to be fluxed out is computed and the same number is transferred across the LES cells. If a fractional number is to be transferred, the LEM cell is split so that exact mass conservation is achieved. It is to be noted that this scalar transport is performed from one
LES cell to the adjacent LES cells only. This is valid as the flow is evolved using sufficiently small time steps.

### 3.2.3.3 Volumetric expansion

In the current implementation of LEM, pressure at sub-grid level is assumed to be same as the resolved pressure. This is a valid assumption as long as there is no fine scale pressure gradient. However, combustion at the sub-grid level increases the temperature and decreases the local density. This decrease in local density results in the non-uniform distribution of volume of the LEM cells. Since the numerical scheme employed in solving LEM equations assumes an uniform-grid and also due to the complexities involved in the programming with non-uniform LEM cells in parallel environment [69], same number of LEM cells should be retained everywhere in the domain. Hence, LEM domain is re-gridded to have cells of equal volume after each splicing [98].

### 3.2.3.4 The large - scale / small scale - coupling

Two way coupling is achieved between the large scales resolved in the LES formulation and the small scales modeled by LEM. The model uses the LES resolved pressure, subgrid kinetic energy, and LES resolved mass flux. It provides to the super-grid level Favre averaged (over the LES cell) values of species mass fractions. Based on those mass fractions, the LES resolved temperature is computed.

In summary, LEMLES performs sub-grid stirring, sub-grid diffusion in a 1D DNS fashion. Thus, the mixing of the scalars is done in an exact fashion, because of which the chemical reaction at sub-grid level will result in more accurate heat release predictions. This heat release causes thermal expansion at the LEM level, that will generate flow motion at the LES level. This transport is very accurately modeled in splicing.
In this chapter, the numerical implementation and the numerical scheme used in solving the filtered Navier Stokes equations (Eq. 17) and the sub-grid kinetic energy equation (Eq. 23) is presented. These equations are solved using a finite-volume approach, the details of which are presented below.

4.1 Finite Volume Scheme

In the finite volume approach, the computational domain is divided into small volumes and the conservation equations (Eq. 17 and Eq. 23) are applied to these control volumes in an integral form:

\[
\frac{\partial}{\partial t} \int_V Q dV + \oint_S (F dS_x + G dS_y + H dS_z) = \int_V \Phi dV
\]  

(44)

where \( V \) is the control volume, \( S \) is the surface, \( F, G, H \) are the flux vectors in \( X, Y \) and \( Z \) directions respectively. \( \Phi \) is the source vector.

Here, \( Q \) is the state vector and \( \Phi \) is the source vector:

\[
Q = \begin{bmatrix}
\bar{p} \\
\bar{p}u \\
\bar{p}v \\
\bar{p}w \\
\bar{p}E \\
\bar{p}k_{sgs} \\
\bar{p}Y_k
\end{bmatrix}, \quad \Phi = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
p^{sgs} - D^{sgs} \\
\bar{\omega}_k
\end{bmatrix}
\]  

(45)

\( F, G, H \) are consists of an inviscid part \( (F_{IV}, G_{IV}, H_{IV}) \), a viscous part \( (F_V, G_V, H_V) \)
and a sub-grid component \((F_s, G_s, H_s)\).

The inviscid fluxes are given by:

\[
F_{IV} = \begin{bmatrix}
    \rho \bar{u} \\
    \rho \bar{u} \bar{u} + \bar{p} \\
    \rho \bar{u} \bar{v} \\
    \rho \bar{u} \bar{w} \\
    \rho \bar{u} (\bar{E} + \bar{p}) \\
    \rho \bar{u} k^{sgs} \\
    \rho \bar{u} Y_k
\end{bmatrix} \quad G_{IV} = \begin{bmatrix}
    \rho \bar{v} \\
    \rho \bar{u} \bar{u} + \bar{p} \\
    \rho \bar{u} \bar{v} \\
    \rho \bar{u} \bar{w} \\
    \rho \bar{v} (\bar{E} + \bar{p}) \\
    \rho \bar{v} k^{sgs} \\
    \rho \bar{v} Y_k
\end{bmatrix} \quad H_{IV} = \begin{bmatrix}
    \rho \bar{w} \\
    \rho \bar{u} \bar{w} \\
    \rho \bar{v} \bar{w} \\
    \rho \bar{w} (\bar{E} + \bar{p}) \\
    \rho \bar{w} k^{sgs} \\
    \rho \bar{w} Y_k
\end{bmatrix}
\]  

(46)

The viscous fluxes are:

\[
F_V = \begin{bmatrix}
    0 \\
    \tau_{xx} \\
    \tau_{xy} \\
    \tau_{xz} \\
    \bar{u} \tau_{xx} + \bar{v} \tau_{xy} + \bar{w} \tau_{xz} - \bar{q}_x \\
    0 \\
    \rho V_{1,k} \frac{\partial \bar{Y}_k}{\partial x}
\end{bmatrix} \quad G_V = \begin{bmatrix}
    0 \\
    \tau_{yx} \\
    \tau_{yy} \\
    \tau_{yz} \\
    \bar{u} \tau_{yx} + \bar{v} \tau_{yy} + \bar{w} \tau_{yz} - \bar{q}_y \\
    0 \\
    \rho V_{2,k} \frac{\partial \bar{Y}_k}{\partial y}
\end{bmatrix}
\]  

(47)

\[
H_V = \begin{bmatrix}
    0 \\
    \tau_{zx} \\
    \tau_{zy} \\
    \tau_{zz} \\
    \bar{u} \tau_{zx} + \bar{v} \tau_{zy} + \bar{w} \tau_{zz} - \bar{q}_z \\
    0 \\
    \rho V_{3,k} \frac{\partial \bar{Y}_k}{\partial z}
\end{bmatrix}
\]

The subgrid fluxes as:
\[ \begin{bmatrix} 0 & \tau_{sx}^{sgs} & \tau_{sx}^{sgs} & \tau_{sx}^{sgs} \\ \tau_{sx}^{sgs} & 0 & \tau_{sy}^{sgs} & \tau_{sx}^{sgs} \\ \tau_{sx}^{sgs} & \tau_{sy}^{sgs} & 0 & \tau_{sy}^{sgs} \\ \tau_{sx}^{sgs} & \tau_{sy}^{sgs} & \tau_{sy}^{sgs} & 0 \end{bmatrix} \quad \begin{bmatrix} 0 & \tau_{sx}^{sgs} & \tau_{sx}^{sgs} & \tau_{sx}^{sgs} \\ \tau_{sx}^{sgs} & 0 & \tau_{sy}^{sgs} & \tau_{sx}^{sgs} \\ \tau_{sx}^{sgs} & \tau_{sy}^{sgs} & 0 & \tau_{sy}^{sgs} \\ \tau_{sx}^{sgs} & \tau_{sy}^{sgs} & \tau_{sy}^{sgs} & 0 \end{bmatrix} \quad \begin{bmatrix} 0 & \tau_{sx}^{sgs} & \tau_{sx}^{sgs} & \tau_{sx}^{sgs} \\ \tau_{sx}^{sgs} & 0 & \tau_{sy}^{sgs} & \tau_{sx}^{sgs} \\ \tau_{sx}^{sgs} & \tau_{sy}^{sgs} & 0 & \tau_{sy}^{sgs} \\ \tau_{sx}^{sgs} & \tau_{sy}^{sgs} & \tau_{sy}^{sgs} & 0 \end{bmatrix} \]

(48)

### 4.2 Domain discretization

To perform the numerical simulation, a computational domain that represents the physical domain is to be specified. Then this computational domain is filled with a set of discrete points on which the governing equations are solved. This set of points is the so-called grid/mesh which plays a prominent role in the evaluation of the above-mentioned fluxes. Two types of grids exist: structured grids, where the grid points follow a particular alignment in all the 3 directions and unstructured grids, where the grid points are on different shapes. In the current study, a butterfly two-domain structured grid is used, the details of which will be provided later.

It is convenient to perform the simulations in a body fitted coordinates. Hence, the physical space \((x, y, z)\) is transformed into a computational space \((\xi, \eta, \zeta)\) using simple chain rules given by Vivian and Vinokur [119].

\[
\begin{align*}
\frac{\partial}{\partial x} &= \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial y} &= \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial z} &= \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta}
\end{align*}
\]

(49)

where \(\xi_x, \eta_x, \zeta_x, \xi_y, \eta_y, \zeta_y, \xi_z, \eta_z, \zeta_z\) are the grid metrics. These matrices represent the ratio of arc lengths in the computational space to that of the physical space. The coordinate transformations are chosen so that the grid spacing in the transformed space is uniform and
of unit length. There is one-to-one correspondence between a physical point and a computational point, except in the regions near the singularities. Applying the transformation to the Navier Stokes equations 44 preserves the nature of the governing equations, but gives rise to new form:

\[ \int_V \frac{\partial}{\partial t} Q' dV + \int_V \left( \frac{\partial F'}{\partial \zeta} + \frac{\partial G'}{\partial \eta} + \frac{\partial H'}{\partial \xi} \right) dV = \int_V \Phi dV \]

where:

\[ Q' = \frac{1}{J} Q \]
\[ F' = \frac{1}{J} \left( \xi_x F + \xi_y G + \xi_z H \right) \]
\[ G' = \frac{1}{J} \left( \eta_x F + \eta_y G + \eta_z H \right) \]
\[ H' = \frac{1}{J} \left( \zeta_x F + \zeta_y G + \zeta_z H \right) \]

where \( J \) is the Jacobian of the coordinate transformation:

\[ J = \frac{1}{\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} \frac{\partial z}{\partial \zeta} + \frac{\partial x}{\partial \zeta} \frac{\partial y}{\partial \eta} \frac{\partial z}{\partial \xi} + \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \zeta} \frac{\partial z}{\partial \eta} - \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} \frac{\partial z}{\partial \zeta} - \frac{\partial x}{\partial \zeta} \frac{\partial y}{\partial \xi} \frac{\partial z}{\partial \eta} - \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \zeta} \frac{\partial z}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \zeta} \frac{\partial z}{\partial \xi}} \]

Here \( J \) can be interpreted as the ratio between the volumes in the computational domain to the physical domain.

4.2.1 Explicit MacCormack Scheme

The numerical solution is advanced in time using a MacCormack explicit predictor-corrector scheme that is second order accurate in time and second-order accurate in space. Explicit scheme is chosen here due to its simplicity in implementation. Even though explicit schemes are less stable and require smaller integration time steps, they are more suitable candidates for reacting simulations. This is due the fact that in reactive calculations, the time steps are determined by the chemical time steps of radicals, which can be very small. An implicit scheme that is easy to implement with bigger time steps looses its advantage in a reacting simulation.

The MacCormack explicit method uses a predictor step that is discretized using either (backward or forward) differencing followed by another corrector step that will be in the reverse order of the predictor step. The idea is to eliminate the bias due to the one sided
differencing and end up with a second order accurate space [63]. It also achieves second order accuracy in time by predicting variable at an intermediate time step in the predictor step and then again predicting variables after $\Delta t$ in the corrector step. The predictor and corrector steps are shown below.

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{2 \Delta x} \left[ (F_{i+1/2,j,k}^{+(n)} - F_{i-1/2,j,k}^{+(n)}) + (G_{i,j+1/2,k}^{+(n)} - G_{i,j-1/2,k}^{+(n)}) + (H_{i,j,k+1/2}^{+(n)} - H_{i,j,k-1/2}^{+(n)}) \right]$$

(53)

$$Q_i^{n+1} = \frac{1}{2} (Q_i^n + Q_i^*) + \frac{\Delta t}{2 \Delta x_{i,j,k}} \left[ (F_{i+1/2,j,k}^{-(*)} - F_{i-1/2,j,k}^{-(*)}) (G_{i,j+1/2,k}^{-(*)} - G_{i,j-1/2,k}^{-(*)}) + (H_{i,j,k+1/2}^{-(*)} - H_{i,j,k-1/2}^{-(*)}) \right]$$

(54)

where * sign denotes the predictor value of the dependent variable and $n + 1$ denotes the corrected value. Also, + denotes the forward differencing and – denotes the backward differencing. Alternating the forward and backward difference in this two time step scheme is equivalent to a central scheme. However, to avoid any bias due to these one sided schemes, the fluxes are computed following some rules [63].

In the above equation, the spatial indices $(i,j,k)$ is a cell center value, whereas $(i + 1/2, j, k)$ is a cell face value. Fluxes are computed at the cell surfaces while the flow information is usually at the center of each cell. Hence, interpolation techniques have to be used to transfer solution from cell center to cell face. In the current work, the following simple flux interpolation is used which ensures a second order accurate scheme.

$$F_{i+1/2}^+ = F_{i+1}$$

(55)

$$F_{i+1/2}^- = F_i$$

(56)

Higher order interpolation schemes can also be used for interpolation [75]. However, these higher order schemes can become unstable and require bigger stencil for computations.
4.2.2 Numerical Time Step

The integration time step is chosen based on the stability requirement of MacCormack explicit scheme. Stability analysis shows that a given information can not travel more than a certain portion of the grid spacing. The information speed is the wave speed and the portion of grid that wave can travel is the Courant-Friedric-Levy (CFL) condition. Wave speed \(v_p\) is based on physical theory and numerical experiments reported in the literature \[63\]. It is taken as sum of the convective \(v_c\), the acoustic \(v_a\) and the diffusive \(v_d\) velocities. The convective velocity is given by the flow velocity, the acoustic velocity is the speed of the sound \(a\) and the diffusive velocity \(v_d\). Thus:

\[
v_c = U \hat{i} + V \hat{j} + W \hat{k}, \quad (57)
\]

\[
v_a = a, \quad (58)
\]

\[
v_d = \frac{2\gamma \mu |d\vec{A}|^2}{\rho Pr V_{i,j,k}}, \quad (59)
\]

where \(Pr\) is the Prandtl number. Note that the expression shown for \(v_d\) is not a true definition, but just a numerical representation. Finally the time step is computed at each point as \([114]\)

\[
\Delta t = \frac{CFL}{\frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} + \frac{|w|}{\Delta z} + a \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} + \frac{2\gamma \mu}{Pr} \left(\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}\right)}} \quad (61)
\]

Note that a single time step is used to evolve the flow for the entire computational domain. Hence the above time step expression is evaluated at every point and then a minimum value over the entire computational domain is used to evolve the flow.

4.3 Boundary Conditions

In the numerical implementation of engineering problems, boundary conditions play an important role in attaining the physically correct solutions. The boundary conditions are specified on the dependent variables along the boundaries of the domain in different ways. These are categorized as follows:
• Dirichlet boundary condition, where the dependent values are specified at the domain boundary.

• Neumann boundary condition, where the normal gradient of the dependent variable is specified at the boundary.

• Mixed boundary conditions, where a combination of Dirichlet and Neumann boundary conditions are specified

The wall boundary conditions and periodic conditions are implemented as:

• No slip conditions at walls, which is the Derichlet type i.e., the normal and tangential velocities at the wall are set to zero

• Adiabatic conditions at walls, which is the Neumann type i.e., the temperature gradient at the wall is set to zero. Also non-catalytic conditions are specified for species mass fractions by setting their gradient to zero.

• Periodic boundary conditions. If the computational domain consists of \( N \) cells from 1 to \( N \), with cells 0 and \( N + 1 \) as boundary conditions, then the periodic conditions are set such that all the dependent variables at cell \( N + 1 \) will be same as that at cell 1 and that all the dependent variables at cell 0 will be same as that at cell \( N \).

The inflow and outflow boundary conditions are much more complicated to implement and require understanding of the wave like behavior possessed by the compressible Navier-Stokes equations. The wave like behavior allows for identification of characteristic waves whose direction and magnitude of propagation can be determined from interior information.

4.3.1 Characteristic boundary conditions

In any subsonic flow, at the boundaries, there are always waves propagating in and out of the domain due to higher wave propagation velocity when compared to flow velocity. Hence, in numerical simulations, where a computational domain is defined, the behavior of these waves must be properly captured to evolve a physically correct solutions. The behavior of outgoing waves can be defined by the solution at and within the boundary, whereas
the incoming wave behavior can be identified based on the conditions present outside the computational domain and hence requires boundary conditions to completely specify their behavior. The above issues are taken into account following the characteristic analysis of Poinset and Lele [86]. Assuming that the characteristic boundary conditions are applied on a boundary located in a $x_2 - x_3$ plane, the characteristic analysis, when used on three dimensional governing Navier-Stokes equation (Eq. 17) provided following equations.

\[
\begin{align*}
\frac{\partial \tilde{\mu}}{\partial t} + d_1 + \frac{\partial \tilde{\mu} u_2}{\partial x_2} &= 0 \\
\frac{\partial \tilde{\mu} u_1}{\partial t} + \tilde{u}_1 d_1 + \tilde{p} d_3 + \frac{\partial \tilde{\mu} u_1 u_2}{\partial x_2} + \frac{\partial \tilde{\mu} u_1 u_3}{\partial x_3} &= \frac{\partial \tau_{11}}{\partial x_j} \\
\frac{\partial \tilde{\mu} u_2}{\partial t} + \tilde{u}_2 d_1 + \tilde{p} d_4 + \frac{\partial \tilde{\mu} u_2 u_2}{\partial x_2} + \frac{\partial \tilde{\mu} u_2 u_3}{\partial x_3} &= \frac{\partial \tau_{22}}{\partial x_j} \\
\frac{\partial \tilde{\mu} u_3}{\partial t} + \tilde{u}_3 d_1 + \tilde{p} d_5 + \frac{\partial \tilde{\mu} u_3 u_3}{\partial x_2} + \frac{\partial \tilde{\mu} u_3 u_3}{\partial x_3} &= \frac{\partial \tau_{33}}{\partial x_j} \\
\frac{\partial \tilde{p}}{\partial t} + \tilde{p} \tilde{u}_1 d_3 + \tilde{p} \tilde{u}_2 d_4 + \tilde{p} \tilde{u}_3 d_5 + \frac{1}{2} \left( \frac{\partial (u_1 \tilde{u}_1)}{\partial x_1} + \frac{\partial (u_2 \tilde{u}_2)}{\partial x_2} + \frac{\partial (u_3 \tilde{u}_3)}{\partial x_3} \right) \\
+ \frac{d_2}{\gamma - 1} + \frac{\partial}{\partial x_2} \left( \tilde{p} \tilde{E} + \tilde{p} \right) \tilde{u}_2 + \frac{\partial}{\partial x_3} \left( \tilde{p} \tilde{E} + \tilde{p} \right) \tilde{u}_3 + (\tilde{\epsilon} - \frac{a^2}{\gamma (\gamma - 1)}) d_1 + \sum_{m=1}^{N} \tilde{p} d_{6+m} + \tilde{p} d_{6+m} + \frac{\partial \tilde{\mu} u_2 k^{gs}}{\partial x_2} + \frac{\partial \tilde{\mu} u_3 k^{gs}}{\partial x_3} \\
+ \frac{\partial}{\partial x_j} \left( \tilde{\mu} u_1 \frac{\partial k^{gs}}{\partial x_j} \right) + P^{gs} - D^{gs} \\
\frac{\partial \tilde{\mu}}{\partial t} + \tilde{\nu} \tilde{d}_1 + \tilde{p} d_6 + \frac{\partial \tilde{\mu} \tilde{u}_2 \tilde{Y}_m}{\partial x_2} + \frac{\partial \tilde{\mu} \tilde{u}_3 \tilde{Y}_m}{\partial x_3} \\
+ \frac{\partial}{\partial x_j} \left( \tilde{p} D_m \frac{\partial \tilde{Y}_m}{\partial x_j} \right) + \tilde{p} \tilde{W}_m, m = 1, N
\end{align*}
\]

where $d_i$ are the various partial derivatives with respect to the $x_1 - $th direction:

\[
\tilde{d} = \begin{pmatrix}
d_1 \\
d_2 \\
d_3 \\
d_4 \\
d_5 \\
d_6 \\
d_{6+m}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial \tilde{\mu} u_1}{\partial x_1} \\
\tilde{p} \frac{\partial \tilde{u}_1}{\partial x_1} + \tilde{u}_1 \frac{\partial \tilde{p}}{\partial x_1} \\
\tilde{u}_1 \frac{\partial \tilde{u}_1}{\partial x_1} + \frac{1}{\tilde{\rho}} \frac{\partial \tilde{\mu}}{\partial x_1} \\
\tilde{u}_1 \frac{\partial \tilde{u}_1}{\partial x_1} \\
\tilde{u}_1 \frac{\partial \tilde{u}_2}{\partial x_1} \\
\tilde{u}_1 \frac{\partial \tilde{u}_3}{\partial x_1}
\end{pmatrix} = \begin{pmatrix}
\frac{1}{\epsilon^2} \left[ L_2 + \frac{1}{2} \left( L_5 + L_1 \right) \right] \\
\frac{1}{2} \left( L_5 + L_1 \right) \\
\frac{1}{2 \epsilon} \left( L_5 - L_1 \right) \\
L_3 \\
L_4 \\
L_6 \\
L_{6+m}
\end{pmatrix}
\]

where $L_i$'s is the characteristic waves amplitude associated with the eigenvalue $\lambda_i$: 50
\[
\tilde{\lambda} = \begin{pmatrix}
\lambda_1 \\
\lambda_2 \\
\lambda_3 \\
\lambda_4 \\
\lambda_5 \\
\lambda_6 \\
\lambda_{6+m}
\end{pmatrix} = \begin{pmatrix}
\tilde{u}_1 - c \\
\tilde{u}_1 \\
\tilde{u}_1 \\
\tilde{u}_1 \\
\tilde{u}_1 + c \\
\tilde{u}_1 \\
\tilde{u}_1
\end{pmatrix}
\]  

(64)

where \(c\) is the speed of sound and:

- \(\lambda_1\) is the velocity of the positive sound wave;
- \(\lambda_2\) is the velocity of the entropy wave (convection velocity);
- \(\lambda_3\) is the velocity of \(\tilde{u}_2\) advection in the \(x_1\)-direction;
- \(\lambda_4\) is the velocity of \(\tilde{u}_3\) advection in the \(x_1\)-direction;
- \(\lambda_5\) is the velocity of the negative sound wave;
- \(\lambda_6\) is the velocity of \(k^{sgs}\) advection in the \(x_1\)-direction;
- \(\lambda_{6+m}\) is the velocity of \(\tilde{Y}_m\) advection in the \(x_1\)-direction, where \(m\) goes from 1 to the number of chemical species considered in the problem.

The amplitudes of the characteristic waves, \(L_i\) are:

\[
\begin{pmatrix}
L_1 \\
L_2 \\
L_3 \\
L_4 \\
L_5 \\
L_6 \\
L_{6+m}
\end{pmatrix} = \begin{pmatrix}
\lambda_1 \left( \frac{\partial \rho}{\partial x_1} - \overline{p} c \frac{\partial \tilde{u}_1}{\partial x_1} \right) \\
\lambda_2 \left( c^2 \frac{\partial \tilde{u}_2}{\partial x_1} - \frac{\partial \overline{p}}{\partial x_1} \right) \\
\lambda_3 \frac{\partial \tilde{u}_2}{\partial x_1} \\
\lambda_4 \frac{\partial \tilde{u}_3}{\partial x_1} \\
\lambda_5 \left( \frac{\partial \overline{p}}{\partial x_1} + \overline{p} c \frac{\partial \tilde{u}_5}{\partial x_1} \right) \\
\lambda_6 \frac{\partial k^{sgs}}{\partial x_1} \\
\lambda_{6+m} \frac{\partial \tilde{Y}_m}{\partial x_1}
\end{pmatrix}
\]  

(65)
Poinset et al, [86] obtained Local One-Dimensional Inviscid (LODI) relations, where the wave amplitude variations in the viscous, three-dimensional Navier-Stokes equations can be inferred:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{1}{c^2} \left[ L_2 + \frac{1}{2} (L_5 + L_1) \right] &= 0 \\
\frac{\partial u}{\partial t} + \frac{1}{2} (L_5 + L_1) &= 0 \\
\frac{\partial e_u}{\partial t} + \frac{1}{2pc} (L_5 - L_1) &= 0 \\
\frac{\partial e_u}{\partial t} + L_3 &= 0 \\
\frac{\partial e_u}{\partial t} + L_4 &= 0
\end{align*}
\]

Based on the LODI equations (66), characteristic boundary conditions at the inflow and the outflow are implemented in this work.

4.3.1.1 Characteristic Subsonic Inflow

For the subsonic inflow in a three dimensional flow with N−species, 5 + N characteristic waves, \(L_2, L_3, L_4, L_5, L_6\) and \(L_6+N\) enter the domain and \(L_1\) leaves the domain at \(\lambda_1 = u_1 - c\). Therefore, the gas density is determined by the flow itself, while all other values are specified. Hence, the inflow conditions are described as:

\[
\begin{align*}
u_1 &= U_{inflow} \\
u_2 &= V_{inflow} \\
u_3 &= W_{inflow} \\
T &= T_{inflow} \\
k_{sgs} &= k_{sgs_{inflow}} \\
Y_k &= Y_{k, inflow} \\
\tilde{d}\tilde{\rho} &= -\Delta t d_1
\end{align*}
\]

where \(\tilde{d}\tilde{\rho}\) is the change in density in \(\Delta t\) and \(d_1\) is computed as:

\[
d_1 = \frac{1}{c^2} \left[ L_2 + \frac{1}{2} (L_1 + L_5) \right]
\]
At the subsonic outflow, a perfectly non-reflecting condition where no incoming waves are allowed can lead to an ill-posedness of the problem [95]. Hence, a partially reflecting conditions are enforced by allowing a pressure wave coming from downstream to enter the computational domain. This is done by imposing $p_\infty$ at the outflow and using this to compute the amplitude of the incoming wave, $L_1$ as:

$$L_1 = \beta (\bar{\rho} - p_\infty)$$  \hfill (69)

where:

$$\beta = \sigma (1 - M^2) \frac{c}{L}$$  \hfill (70)

and $M$ is the maximum Mach number in the flow, $L$ is a characteristic length of the domain, $c$ is the speed of the sound and $\sigma$ controls the reflection of the waves. A value of $\sigma = 0.15$ is used in this study. The specification of $L_1$ just sets only one physical boundary conditions. All the other dependent variables at the boundary is estimated by solving the system of conservation equations using an upwind backward differencing scheme to compute the gradients.

## 4.4 Linear Eddy Mixing Model Implementation

This section describes the numerical implementation of the linear eddy mixing (LEM) model in the LES solver. The implementation is such that LEM can be used like a black box. What it means is that LEM solver can be used with any LES flow solver without modifying the LEM as such. However, the flow solver must adhere to certain restrictions such as explicit schemes (Implicit schemes can be very expensive in terms of memory requirement) and low dissipation schemes (numerical dissipation kills physical processes such as turbulence which makes LEM invalid). LEM requires sub-grid turbulent kinetic energy ($k_{sgs}$), super grid pressure and the mass flux through each LES face. And it solves the unfiltered scalars (temperature,species) equation. The evolved scalar field is provided to the LES solver. Note that, in the current implementation of LEM, the LES solver only gets the species field from LEM solver. Temperature is evolved inside LEM solver, but is not used in the LES solver.
However, the temperature evolved within LEM and the resolved temperature in LES differ by only 2%. The reason is that the temperature evolved inside LEM neglects the pressure work (note the equation 38). Within LEM, the main processes solved are the (1) reaction diffusion equation and (2) the splicing or the large scale convection process.

4.4.1 The reaction diffusion equation

In the reaction - diffusion Eq. 39 four distinct phenomena are solved at their own time scales. The processes and their time scales are described below.

A. Molecular diffusion.

This is the slowest process and is associated with diffusion of species and temperature. The time scales associated with this process will be the largest among all the processes [97]. The diffusion time is given by

$$t_{\text{diffusion}} = \frac{s^2}{\kappa \max(D_k)}$$  \hspace{1cm} (71)

where $s$ is the LEM grid size, $D_k$ is the diffusion coefficient of species $k$ and $\kappa$ is a model constant, set here to 0.25 for reasons of numerical stability [97].

B. Chemistry.

This time scale, $t_{\text{chem}}$, is associated to the rate at which species are converted in a chemical reaction. It is usually the smallest time scale [97] in the flow unless the turbulent time scales compete with the chemical time scales. The current study uses a chemical time step $N$ times smaller than the molecular diffusion time scale, $t_{\text{diffusion}}$. The value of $N$ changes with the application as well as the employed chemical kinetics. More details on this will be provided later.

C. Thermal expansion.

The time scale is associated with the volumetric expansion induced by the increase in temperature through chemical heat release. Ideally thermal expansion happens soon after the heat release. But in the current implementation $t_{\text{vol}}$ is set to be equal to the $t_{\text{diffusion}}$ for the reasons of numerical stability [97].

D. Turbulent stirring.
The turbulent stirring time scale is associated to the turbulent convection by small (subgrid) eddies and is defined by:

\[ \tau_{stir}(x) = \frac{1}{\lambda \Delta} \]  

(72)

where \( \lambda \) is the turbulent stirring frequency, given by Eq. 43.

This is the time scale at which the triplet maps are implemented. It is a strong function of sub-grid Reynolds number \( Re_\Delta \), i.e., higher \( Re_\Delta \) implies a smaller stirring time scale.

The length of the LEM domain (\( L^{LEM} \)) depends on the LES grid size as:

\[ L^{LEM} = \frac{\Delta V_{LES}}{N^{LEM}} \]  

(73)

where \( N^{LEM} \) is the number of LEM cells per LES cell and \( \Delta V_{LES} \) is the volume of the LES cell. For the linear eddy mapping to work, at least 6 LEM cells are needed inside the LES cell. In addition, \( N^{LEM} \) must be a multiple of 3.

All the above processes are explicitly solved on a 1D sub-grid domain within each LES cell. The solver uses an operator splitting method [105, 14] which allows for resolution of the chemical, diffusion and turbulent processes at their respective time scales. Thus, at each LES time step the diffusion and stirring time scales are determined. Depending on whichever is the smallest time scale (usually its the stirring time scale), that process is first solved. Sometimes if the stirring time is so low, then a couple of stirrings are performed within one diffusion time step. In addition, the technique also allows for a more (> 1) number of diffusion steps if the diffusion time step is lower than the LES time step. Since, the LES time step is based on flow acoustics, it is usually the smallest time step in the flow. In such a case, only one stirring and diffusion step is performed. The chemical species source terms are determined by integrating over the diffusion time step. The thermal expansion is implemented after every diffusion step.

4.4.2 The splicing algorithm

In LEM, the reaction diffusion equation is first solved and only then a lagrangian convection of LEM scalar fields is performed across LES cells. This is achieved using splicing algorithm
at each LES time step. Splicing involves transfer of LEM cells between adjacent LES cells using the LES resolved mass flux. The adjacent cell assumption is valid here as the time steps at which flow is evolved is very small (order of $10^{-8}$). At these small time steps, species will most likely move from one LES cell to only its adjacent cell. Also, the small time steps only allow transfer of partial LEM cells between adjacent cells.

The numerical implementation of splicing is as follows. Splicing requires the information of the absolute mass flux across each face for every LES cell from the LES solver. This flux is converted into absolute mass at each of the faces. This is the mass that can either go out or come in through this face. This mass is first sorted out based on the sign convention proposed by Chakravarthy and Menon [18]. The sorting is done to identify the order of the 3D advection process. The largest negative flux will be the first one to exit the LES cell. The absolute mass is also converted to an equivalent number of LEM cells. Based on the direction of the mass flux, equivalent number of LEM cells is transferred between the LES cells. This procedure is represented in the 2D in Fig. 7. Further details on the splicing numerical procedure are given by Sankaran [97]. Finally, the re-gridding procedure is carried out to ensure uniform LEM grid resolution and constant number of LEM cells in all LES cells. The uniform grid resolution is not a requirement in LEM, but it is done to avoid programming complexities in parallel environment.
CHAPTER V

PROBLEM SETUP

5.0.3 SPRF geometry

The SPRF combustor along with its characteristic dimensions is shown in Fig. 8. The apparatus consist of three main components: a combustor, an injector and an air/fuel supply system. The combustor is a cylindrical quartz tube (4) wrapped with thermal insulation, and closed on one side with an end plate (6) (stagnation end). The injector is the centrally located dual concentric tube at the open end (opposite to the end plate). In the non-premixed mode, fuel flows through the central tube (2) and air flows through the concentric outer tube. The same combustor is also operated in the premixed mode by simply shutting off the fuel supply (1), and by discharging the premixed mixture through the outer tube. The central tube (2) is shut off far upstream. The outflow (4) is through a larger annular region that surrounds the injection system.

5.0.4 Computational domain

To perform simulations on the SPRF combustor, a computational domain must be considered. For the current simulations, the computational domain used is shown in Fig. 9. The

![SPRF geometry](image)

Figure 8: SPRF geometry
domain is chosen so as to include all the geometric features that can influence the flow field inside the combustor. As an example, in the premixed case, the central tube was shut off far upstream. This creates a cylindrical cavity, that effects the near field field. Hence it is included in the computations. However, to reduce the computational cost, the length of the cylindrical cavity is restricted to be equal to the length of the injector.

5.0.5 Simulated conditions

(table needed) In the premixed mode, both non-reacting and reacting cases are simulated. For the non-reacting case, air at atmospheric pressure and room temperature is injected into the combustor at a volumetric flow rate of 0.00638 $m^3/s$. In the reacting case, a premixed mixture of methane and air with a net flow rate of 0.00676 $m^3/s$ (give in terms of mass flow rate) and lean equivalence ratio of $\phi = 0.58$ is injected into the combustor. The conditions chosen are away from the lean blow out limit of $\phi = 0.48$. Using the flow rate, a bulk velocity of 69.3 $m/s$ is obtained in the non-reactive case.

In the premixed reactive case, there is preheating of the reactant jet flowing through the annular injector by the reverse flow of the hot products flowing over this annular injector. It is reported [11] that the jet is preheated to 500 $K$ before reaching the tip of the injector. Note that the above flow rates for the room temperature conditions. Due to preheating, the flow rate changes, but the mass flow rate will be same as that at the room temperature conditions.
By increasing the temperature and the velocity, the above conditions can be matched. In
the current premixed work, the preheating effect is included in the computations by setting
the temperature and the bulk velocity of the inflow jet at 500 K and 129 m/s respectively.
Also random inflow turbulence with a RMS velocity profile with peak intensity of 15 % is
superimposed on the mean velocity profile in all the directions. In addition, a profile of
sub-grid kinetic energy is also imposed at the inflow. For cold flow, the Reynolds number
based on the inlet bulk velocity and the annular injector width is \(12.9 \times 10^3\), while the sub-
grid Reynolds number based on the simulated \(k_{sgs}\) in the shear layer close to the injector
is around 354. Similarly, for the hot flow, the Reynolds number and the sub-grid Reynolds
number are computed and they are found to be 9820 and 304, respectively.

Reacting non-premixed case is also simulated in the SPRF configuration. In this case,
air with a flow rate of 0.00638 \(m^3/s\) and fuel with a flow rate of 0.00038 \(m^3/s\) are injected
through the annular and central tubes respectively. The overall equivalence ratio is 0.58.
The preheating effect is included in the computations by setting the temperature and bulk
velocity of the air at 450 K and 104 m/s. Fuel is assumed to be injected at temperature
lower than 450 K. The Reynolds number at the annular inflow based on the annular injector
width is 10160, while the Reynolds number at the fuel inlet based on central tube diameter
is 7680. In the regions of high turbulence, the sub-grid Reynolds number is around 274.

The above details are also provided in the Table 1.

**5.0.6 Boundary conditions**

The boundary conditions used here are characteristic conditions of Poinso and Lele [86].
For the inflow, the density is determined by the flow itself, while all the other values
\((u_1, u_2, u_3, T, k_{sgs}, Y_m)\) are specified. A 1/8 turbulent velocity profile has been imposed
at the annular injector. The analytic expression of the velocity profile \((u_a)\) is given by:

\[
u_a = u_{amax} \left[ 1 - \frac{abs \left( r - \frac{r_1 + r_2}{2} \right)}{r_2 - r_1} \right]^8 \tag{74}
\]

while for the non-premixed case, the fuel velocity profile \((u_f)\) is given by:

\[
u_f = u_{fmax} \left[ 1 - \frac{r}{r_1} \right]^8 \tag{75}
\]
Table 1: Flow conditions. Flow rates is in $m^3/s$, temperature in $K$, velocity in $m/s$, $Re_a$ is based on annular injector width and annular jet inflow bulk velocity, $Re_c$ is based on central tube’s dia and fuel inflow bulk velocity, $Re_\Delta$ is local maximum sub-grid Re based on the simulated $k_{sgs}$ and LES filter width in the shear layer.

<table>
<thead>
<tr>
<th></th>
<th>Non-reacting premixed</th>
<th>Reacting premixed</th>
<th>Reacting non-premixed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annular jet flow rate</td>
<td>0.00638</td>
<td>0.00676</td>
<td>0.00638</td>
</tr>
<tr>
<td>Central jet flow rate</td>
<td>-</td>
<td>-</td>
<td>0.00038</td>
</tr>
<tr>
<td>Annular jet temperature</td>
<td>300</td>
<td>500</td>
<td>450</td>
</tr>
<tr>
<td>Central jet temperature</td>
<td>-</td>
<td>-</td>
<td>330</td>
</tr>
<tr>
<td>Annular jet bulk velocity (with preheating)</td>
<td>-</td>
<td>122</td>
<td>104</td>
</tr>
<tr>
<td>Equivalence ratio ($\phi$) (effective)</td>
<td>-</td>
<td>0.58</td>
<td>0.58</td>
</tr>
<tr>
<td>Annular injector Re ($Re_a$)</td>
<td>12,900</td>
<td>12,900</td>
<td>10,160</td>
</tr>
<tr>
<td>Central jet Re ($Re_c$)</td>
<td>-</td>
<td>-</td>
<td>7,680</td>
</tr>
<tr>
<td>sub-grid Re ($Re_\Delta$)</td>
<td>354</td>
<td>304</td>
<td>274</td>
</tr>
</tbody>
</table>

where $r_1$ and $r_2$ are the radii of central tube and the inner radii of the annular injector respectively. Only the $u_1$ component is set using the above relations. Both $u_2$ and $u_3$ are zero at the inflow.

At the outflow, partially reflecting conditions are enforced by allowing a pressure wave coming from downstream to enter the computational domain. Details of the procedure for setting these conditions can be found in chapter 4. On all the solid walls, no-slip, adiabatic and non-catalytic conditions are prescribed.

5.0.7 Grid

The computational domain is resolved using a two-domain butterfly grid. Different grid sizes are first tested in the non-reacting case to identify the most appropriate grid for the LES. Table 2 shows the different grids that are used in the study. The results from these studies are not shown here. However, to demonstrate the improvements with increase in grid size, radial profiles of mean and RMS of axial velocity at 57 and 113 $mm$ from the injector is shown in Fig. 10. Clearly, the coarse grid is not capturing both mean and RMS. The finest grid resolves the both the quantities. Hence, this grid is chosen for all the simulations. This section only describes the finest grid.
(a) Radial profiles of mean axial velocity at two axial locations using Grid 1 and Grid 4

(b) Radial profile of RMS of axial velocity at two axial locations using Grid 1 and Grid 4

**Figure 10:** Comparison of Mean and RMS of axial velocity
Table 2: Different grids employed in the non-reacting studies

<table>
<thead>
<tr>
<th>Grid</th>
<th>Domain 1</th>
<th>Domain 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid 1</td>
<td>92X75X57</td>
<td>92X15X15</td>
</tr>
<tr>
<td>Grid 2</td>
<td>112X75X57</td>
<td>112X15X15</td>
</tr>
<tr>
<td>Grid 3</td>
<td>132X81X57</td>
<td>132X15X15</td>
</tr>
<tr>
<td>Grid 4</td>
<td>194X75X57</td>
<td>194X15X15</td>
</tr>
</tbody>
</table>

The finest grid (Grid 4) consists of a cartesian grid of $194 \times 15 \times 15$ in the central portion of the combustor a body-conforming grid of $194 \times 75 \times 51$ surrounds this central Cartesian grid. The grid is non-uniform and is clustered near regions of high gradients. The resolution is around $y^+ = 15$ near the walls of the injector. The $y^+$ is calculated based on empirical relations for wall skin friction coefficient ($C_f$), wall shear stress ($\tau_w$) and friction velocity ($u^*$) for a circular duct [30]. With this resolution, nearly 15 points are in the outer shear layer width, which is shown to be adequate [70]. The axial grid is clustered near the injector with $\Delta x = 0.2mm$ at the injector tip. It is then stretched after one jet diameter downstream. The grid stretching is less than 5% in the near field region, and stretching increases to a maximum of around 10% far away from the injector.

The grid is justified for the premixed non-reactive studies by studying the spectra of the resolved turbulent kinetic energy contained in the axial velocity component, $E_{1,1}$. The location chosen is in the shear layer and is located at a axial distance of 22 $mm$ from the injector and radius of 4 $mm$. The computed energy spectrum shown in Fig. 12 follows the Kolmogorov’s $-5/3$ law for at least one decade. This is considered reasonable for LES. In the case of LEMLES computations, no further grid refinement is required due to the sub-grid approach. Hence the above spectrum will be be sufficient to show that the grid is reasonable for the premixed reacting case.

The spectrum shown in the Fig. 12 does not show an indication of the frequency of the vortex shedding. To visualize vortex shedding in the present setup, a $Q$ criterion [102] is computed using the instantaneous velocity field. The large scale coherent structures can be visualized by showing a positive isovalue for $Q$, which is computed as:

$$Q = \frac{1}{2}(\Omega_{ij}\Omega_{ij} - S_{ij}S_{ij})$$  \hspace{1cm} (76)
(a) Isometric view with grid shown on the center-line plane cut

(b) Grid resolution close to the injector

(c) Butterfly grid

Figure 11: Computational grid
where $S_{ij}$ and $\Omega_{ij}$ are, respectively the symmetric and anti-symmetric strains. Figure 13 shows the isocontour of $Q$, which shows a roll up of azimuthal vortical structures very near to the injector. Typically in a free turbulent jet, these structures grow by pairing and develop into large three dimensional structures [24]. This does not seem to happen in the SPRF combustor. The azimuthal vortices break up and disappear completely within the first 10 jet diameters. This could be due to the presence of reverse flow in this setup.

The LEM grid inside each LES cell should be able to resolve $\eta$ in LEMLES. This sub-grid structure within each LES cell is resolved using 12 LEM cells in both premixed and non-premixed reacting cases. The justified for this in the premixed reacting case is given below. Note that further justification for the non-premixed case is not required as the highest sub-grid Reynolds number (which determine the sub-grid resolution) is lower in the non-premixed case (refer Table 1.

Using Kolmogorov's scaling law and the simulated $k^*\eta^*$ (on the LES grid) values of the non-reactive jet, the Kolmogorov scale $\eta$ evaluated in regions of high turbulence is found to be around 0.06$mm$. Based on this Kolmogorov scale, 12 LEM cells in each LES cell is found to be adequate to resolve $\eta$. Also, CHEMKIN PREMIX package is used to perform
Figure 13: Visualization of coherent structures downstream of the injector using the iso-
surface of $QU_0^2/D_0^2 = 2 \times 10^9$.

Laminar flame speed calculations with the conditions present in SPRF combustor. The
calculations showed that the ratio of flame thickness to Kolmogorov’s scale to be around 30
in the regions of interest. This means that flame is resolved with approximately 30 LEM
cells (one LEM cell $\approx \eta$). In other words, flame is resolved with 3 cells at the LES level.
Also, in a typical lean premixed system (without preheating, dilution), the reaction zone
thickness is 1/10 of the flame thickness [85]. Hence the simulations are able to resolve the
reaction zone with 3 LEM cells.

5.0.7.1 LDKM model coefficients

The turbulence model is based on the transport equation of the sub-grid turbulent kinetic
energy (TKE). To compute sub-grid TKE, the turbulent viscosity and turbulent dissipation
are determined locally using the local grid size and the sub-grid turbulent velocity obtained
from sub-grid TKE. The model coefficients $C_\nu$ and $C_\varepsilon$ represent these turbulent viscosity and
turbulent dissipations respectively. The instantaneous values of these coefficients obtained
Figure 14: Instantaneous contours of the LDKM coefficients predicted by the LEMLES.

from LEMLES simulations are shown in Fig. 14. Both the coefficients vary significantly over the entire domain. This suggests that the dynamic evaluation of these coefficients is a requirement in the simulations. In addition, high $C_\nu$ also represent high turbulent viscosity in the flow. It is also observed that in most of the regions, $C_\nu$ in the shear layers is close to the mean value of 0.067. The dissipation coefficient is highest in the stagnation zone due to the presence of walls.
5.0.8 Chemical kinetics

In the current simulations, two different mechanisms are used to compute the reaction rates. The first mechanism is a four-step, seven-species reduced chemical mechanism, consisting of the two-step Westbrook and Dryer [121] methane-air mechanism and a two-step NO chemistry involving thermal and non-thermal NO formation [78]. The NO rate for the thermal route is computed as $10^{2.946T^{-0.5}} e^{-68899.0/T} N_2O_2$, while for the non-thermal route is computed as $10^{14.967e^{-53369.0/T}} CO_0^{0.7211O_2^{0.0111}}$. The methane oxidation steps are as follows:

$$CH_4 + \frac{3}{2}O_2 + 3.76N_2 \rightarrow CO + 2H_2O$$  \hspace{1cm} (77)
$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$  \hspace{1cm} (78)

The second mechanism is a 16 species, 12 steps, methane reaction mechanism [112]. The reaction steps are:

$$O_2 + 2CO \leftrightarrow 2CO_2$$
$$H + O_2 + CO \leftrightarrow OH + CO_2$$
$$H_2 + O_2 + CO \leftrightarrow H + OH + CO_2$$
$$HO_2 + CO \leftrightarrow OH + CO_2$$
$$O_2 + H_2O_2 + CO \leftrightarrow OH + HO_2 + CO_2$$
$$O_2 + 0.5C_2H_2 \leftrightarrow H + CO_2$$
$$O_2 + CH_3 + CO + C_2H_4 \leftrightarrow CH_4 + CO_2 + CH_2O + 0.5C_2H_2$$
$$O_2 + 2CH_3 \leftrightarrow H_2 + CH_4 + CO_2$$
$$O_2 + 2CH_3 + CO \leftrightarrow CH_4 + CO_2 + CH_2O$$
$$O_2 + CH_3 + CO \leftrightarrow H + CO_2 + CH_2O$$
$$O_2 + CO + C_2H_6 \leftrightarrow CH_4 + CO_2 + CH_2O$$
$$H + OH \leftrightarrow H_2O$$  \hspace{1cm} (80)

Two premixed cases were simulated; one with the simple kinetics and the other with the detailed chemistry, while the non-premixed simulation was performed using a one step global mechanism [121].

67
5.0.9 Direct source term estimation

In LEMLES, computing the reaction rates using direct integration of the reaction rate equation using an ordinary differential solver (e.g., DVODE package) is proved to be prohibitive. Even though this approach has maximum accuracy, it becomes extremely expensive for complex mechanisms. To reduce the computational costs, Eggenspieler and Menon [27] decoupled chemistry from the diffusion time scales and evaluated the chemical source term at smaller time scales than the diffusion time step. This method called as Direct Source Term Estimation (DSTE) is implemented in the present studies. The diffusion time step is divided into 4 sub time steps and the reaction rates are computed at each of these sub time steps. The accuracy of the computed rates is determined by comparing with that of the rates computed using the DVODE package. In the case of SPRF combustor simulations with the simple kinetics, the difference between the reaction rates using the above two approaches is found to be less than 10% throughout the combustor. Considering that the simulations are 3D in nature and that the speed-ups obtained using DSTE are close to 3 times compared to using DVODE package, the accuracy of the calculation of reaction rates is adequate. The speed up factors obtained by using the DSTE method is shown in Table 3. In the case of the complex chemistry, the number of sub time steps used is 10 [90].

In both EBULES and TFLES approaches, the reaction rates are evolved only once in every LES time step.

Table 3: Speedup factors for different methods of estimating the chemical source terms. DVODE = Direct integration of the reaction rate equation using an ordinary differential solver; DSTE1 = Direct estimation of the Arrhenius reaction rate at the LES time scale; DSTE2 = Direct estimation of the Arrhenius reaction rate at a time scale 2 times smaller than the LES time step; DSTE4 = Direct estimation of the Arrhenius reaction rate at a time scale 4 times smaller than the LES time step; DSTE10 = Direct estimation of the Arrhenius reaction rate at a time scale 10 times smaller than the LES time step;

<table>
<thead>
<tr>
<th>Method</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>DSTE 1</td>
<td>1.000</td>
</tr>
<tr>
<td>DSTE 2</td>
<td>1.1</td>
</tr>
<tr>
<td>DSTE 4</td>
<td>1.9</td>
</tr>
<tr>
<td>DSTE 10</td>
<td>5.8</td>
</tr>
<tr>
<td>DVODE</td>
<td>6.03</td>
</tr>
</tbody>
</table>
5.0.10 Computational costs

The sub-grid approaches used in the study are the EBULES, TFLES and LEMLES. One of the factors that restricts the choice of these approaches is the computational costs of the simulations. Approaches such as EBULES are used mainly because of their computational efficiency. A series of tests are performed to study the efficiency of each of these approaches in SPRF configuration. The tabulated costs are shown below.

**Table 4:** Speedup factors for different combustion closures with global one step kinetics and detailed chemistry (80). $DSTE1 =$ Direct estimation of the Arrhenius reaction rate at the LES time scale;

<table>
<thead>
<tr>
<th>Method</th>
<th>Speedup one step</th>
<th>Speedup detailed kinetics</th>
</tr>
</thead>
<tbody>
<tr>
<td>EBULES</td>
<td>1.000</td>
<td>14.13</td>
</tr>
<tr>
<td>TFLES</td>
<td>1.04</td>
<td>no validity</td>
</tr>
<tr>
<td>LEMLES DSTE1</td>
<td>3.7</td>
<td>121.65</td>
</tr>
</tbody>
</table>

5.0.11 Numerical issues

Large eddy simulations are more vulnerable to numerical instabilities while performing the practical calculations. The primary reasons being the use of low order schemes and the under-resolution of the flow. Such numerical instabilities are also encountered in the simulations of the non-premixed mode of combustion in SPRF. In this mode, fuel and air enter into the combustor separately and are allowed to mix inside the combustor. The extent of mixing is defined in terms of the a dilution length, defined as the axial distance by which the fuel jet dilutes to a specified concentration level. It was mentioned in chapter 2 that this dilution length is a function of ratio of jet velocities. Lowering the ratio of fuel velocity with respect to air jet velocity decreases the dilution length and hence the mixing. Therefore, it is natural to have very high air jet velocity in combustor applications. This increases the strain rates between the fuel and air shear layers. Resolution of this highly intensive mixing is one of the major concern in the computations.
The above problem can be described in the current numerical setup as follows. Consider two adjacent LES control volumes in the highly mixing region. With the evolution of flow in time, a situation can occur where there is some fuel in one LES cell volume and the adjacent cell has no fuel present in it. In such a situation, consider the computation of convective energy gradient ($\partial EU/\partial x$). The total energy $E$ consists of the chemical energy that appears as the heat of formation (or bond energy), the sensible energy, the resolved kinetic energy and the sub-grid kinetic energy. Among all these, the chemical energy values are usually the highest component (order of $10^7$). Hence, in the above encountered situation, the cell which has fuel (which carries the chemical energy) has very high $EU$ value if the velocity at that cell is also high, while the adjacent cell which has no fuel, the chemical energy component is zero. Hence, the gradient of the $EU$ between these two cells is very high. To resolve such gradients in the SPRF combustion, the grid requirement is very high and performing LES on such grids is computationally very expensive. These situations are always encountered in the SPRF configuration. The numerical scheme used in the current studies is the predictor corrector MacCormack scheme which is second order accurate both in space and time. This scheme being a low dissipative scheme could not handle such discontinuities in the flow.

A typical remedy for the above situation is to incorporate some form of artificial dissipation (Jameson dissipation or upwind biased schemes or explicit filtering schemes). Unfortunately, these approaches can lead to unwanted damping of physical processes and can cause numerical errors. However, without resorting to schemes that introduce artificial dissipation, the numerical instabilities as described above can be eliminated using a different form of the energy equation. Instead of total energy, when a non-chemical energy (Total energy - chemical energy) is solved, the instabilities are completely eliminated. Although not presented here, the solution with sensible energy equation are without numerical errors in the conventional LES approaches such as EBULES and TFLES in the non-premixed mode. The filtered form of sensible energy equation is shown below. The right hand side of the equation includes the source terms which is different from that of the total energy.
\[
\frac{\partial \tilde{\rho} \tilde{E}_{NC}}{\partial t} + \frac{\partial}{\partial x_i} \left[ (\tilde{\rho} \tilde{E}_{NC} + \tilde{p}) \tilde{u}_i + \tilde{q}_{NC,i} - \tilde{u}_j \tilde{\tau}_{ji} + H_{NC,i}^{s g s} + \sigma_i^{s g s} \right] = \sum_{k=1}^{NS} - \Delta \tilde{h}_{f,k} \tilde{w}_k \tag{81}
\]

where \(NS\) is the total number of species and

\[
\tilde{E}_{NC} = \sum_{k=1}^{NS} c_{v,k} \tilde{Y}_k \tilde{T} + \frac{1}{2} \tilde{u}_i \tilde{u}_i + k^{s g s} \tag{82}
\]

\[
\tilde{q}_{NC,i} = -k \frac{\partial \tilde{T}}{\partial x_i} + \tilde{\rho} \sum_{k=1}^{NS} c_{p,k} \tilde{Y}_k \tilde{V}_{i,k} \tag{83}
\]

\[
H_{NC,i}^{s g s} = -\tilde{\rho} \frac{\nu_l}{\tau_l} \frac{\partial \tilde{H}_{NC}}{\partial x_i} = -\tilde{\rho} \frac{\nu_l}{\tau_l} \frac{\partial}{\partial x_i} \left( \sum_{k=1}^{NS} c_{p,k} \tilde{T} + 0.5 \tilde{u}_i \tilde{u}_i + k^{s g s} \right) \tag{84}
\]

Note that the source term appears on the right hand side.

In the present work, LEMLES approach is used to simulate the non-premixed combustion. As described earlier, the scalars are evolved in a separate manner than the LES equations. In such a case, the sensible energy equation calculation added more numerical errors. The primary reason is due to the inconsistency in the formulation of LES and LEM equations. Due to these issues, the current work uses an explicit filtering in the regions where the above type of situations are encountered.
CHAPTER VI

VALIDATIONS OF PREMIXED CASES

This chapter provides validations of the non-reacting and the reacting studies of the pre-
mixed mode in the SPRF combustor. The following issues will be addressed.

- Validation of non-reactive LES results with experimental data.
- Validation of reactive LES results in the premixed mode with experiments. Here
  the applicability of different turbulent chemistry closures will also be demonstrated.
  Simple chemical kinetics given in EU. 77 is implemented in all the simulations
- Showing that LEMLES without any modification to the earlier versions describes the
  flow thermal behavior in the premixed mode.
- Validation LEMLES calculations using detailed chemical kinetics given in Eq. 80.

6.1 Non-reacting studies

The time averaged data for 6 τ (τ defined earlier) is presented here. The PIV data showed
here is averaged over 300 instantaneous PIV images sampled at a frequency of 10 Hz [34].
The grid used for PIV is uniform with volume 2.19X2.19X0.6 mm³.

Figure 15 shows the variation of the mean axial velocity along the center-line of the
combustor. The plot shows the mean axial velocity along the y-axis and the axial distance
(x) along the x-axis. The flow is from the left to the right and x = 0 corresponds to the
exit plane of the injector. Along the centerline, the annular jet is slowed down by the
presence of the cylindrical cavity present inside the central tube. The cavity causes a small
recirculation bubble in front of the center tube. As we move downstream, the outer shear
layer of the annular jet merges and the flow accelerates to a peak velocity of 67 m/s. The
axial velocity decays beyond this location. It should be noted that the velocity decay is
very well predicted by the LES results. Overall, there is a very good agreement between
the time-averaged LES and PIV data. In the same plot, the velocity decay computed using free jet [91] and a confined jet [60] models are also shown. The velocity decay in the free jet model is given as $6.3d/x$ and that in the confined jet model is $6.3d/x - 1.4d/D$, where $d$ is the injector diameter and $D$ is the confined tube diameter. Typically $x$ is measured from a virtual origin. Here the virtual origin is considered as the injector exit. The peak velocity ($U_o$) used in the models is 67 $m/s$. The centerline decay in the SPRF combustor and the free jet model can be overlapped if the constant 6.3 is lowered and the virtual origin is changed. Also, lowering the peak velocity can provide a better match. There is an initial region between 50 and 75 $mm$ from the injector, where the velocity gradient is constant. This shows a free jet like behavior in this region. Further downstream, between 60 $mm$ and 150 $mm$ from the injector, the confined jet model overpredicts the velocity. The deviations of the model are due to the reverse flow caused by the stagnation end plate. Thus, it can be observed from figure 15 that the centerline decay in SPRF resembles that of a free jet near the injector, and a confined jet influenced by the reverse flow (due to the stagnation end plate) in the rest of the combustor.

Figure 16 shows the comparison between LES and PIV data of the mean axial velocity profiles at four axial locations; $x = 57, 113, 187$ and 245 $mm$. The figure shows the radial variation of the velocity at these locations, with velocity plotted on the $x$-axis and radial distance along the $y$-axis. The flow is from the left to the right. The velocity profiles in the combustor look similar to that of the velocity profiles in a confined jet. The comparison of the LES results with the PIV data shows good agreement. The computations exhibit more symmetry than the measurements, and measured asymmetry is likely due to the slight misalignment of the inner tube within the annular injector [35]. Near $x = 57$ and 113 $mm$ from the injector, both LES and PIV indicate significant reverse flow close to the combustor walls. This causes a rapid growth of the mixing layer in this region, which saturates after approximately half the length of the combustor. After this point, the flow around the center-line of the combustor is effected by the presence of the stagnation region and slows down, resulting in a more uniform velocity profile near the stagnation end of the combustor.

Figure 17 shows the comparison of RMS axial velocity profiles at four axial locations
in the combustor. This plot is generated in the same way as Fig. 16. Note that LES only shows the resolved part of the turbulence intensities. The agreement between PIV and LES are quite satisfactory near the injector and shows very little discrepancy downstream of the combustor. Both LES and PIV show a spread of RMS levels at $x = 113 \text{ mm}$. This accurate prediction of the spread of RMS is attributed to the fine resolution of the grid that was shown to resolve the inertial range length scales in Fig. 12.

It should be noted that the current simulations employed a turbulence model based on the transport equation of the turbulent kinetic energy, which accounts for the non-equilibrium (turbulence production and dissipation can be different) effects in the flow. This feature, together with the elimination of the use of any ad hoc coefficients ($C_p$ and $C_e$), resulted in LES being able to resolve the relevant flow features with good accuracy, as shown in Figures 15, 16.

### 6.2 Reactive jet - simple kinetics

The reacting flow is simulated with three different approaches; EBULES, TFLES and LEMLES (defined earlier). These approaches differ primarily in the way in which the turbulence chemistry interactions are implemented. Among these approaches, EBULES and TFLES are the conventional closures at the LES resolved scales, whereas LEMLES provides closure directly at the sub-grid scales. In the following sections, simulation results obtained from all these approaches are compared with the experimental data. Both the EBULES and TFLES simulations were run for $6 \tau$ whereas LEMLES simulations were run for $4 \tau$.

#### 6.2.1 Time averaged results

Figure 18 shows the heat release in the SPRF combustor. The heat release is obtained in the experiments by the chemiluminescence technique [34] and in computations by employing different turbulence-chemistry closures. In the experiments, the chemiluminescence field shown is the line of sight time averaged data. In the computations, a similar line of sight time averaged procedure is performed on the heat release, which is obtained using the
expression:

\[
\sum_{k=1}^{N} \overline{w_k} \Delta h_{f,k}
\]  
(85)

where, \( \overline{w_k} \) is the mean reaction rate of species \( k \), \( \Delta h_{f,k} \) is the heat of formation of species \( k \) and \( N \) is the total number of species. In the figure, the injector is located at the top and the flow is from the top to the bottom. The LEMLES predictions are visually closest to the experimental results. EBULES could not predict any defined flame structure due to its simplistic nature. The EBULES approach (even though computationally efficient) has some well known limitations. For example, the model uses \textit{ad hoc} constants to compute the mixing time. It is limited in its capability to predict the right heat release rates, and hence the other combustion characteristics in the SPRF setup. The other computationally efficient TFLES approach is able to capture a defined flame structure, however, the predicted flame length is longer than the measurements. In TFLES, efficiency functions (denoted as \( E \) in Eq. 32) are needed to include the sub-grid effects on the flame. These functions are derived using DNS studies for the specific kinetics. Hence, the functions can vary depending on the chemical kinetics employed. In the current TFLES implementation, the functions are taken from the DNS studies by Colin et al. [21]. However, the chemical mechanism employed here is different from that used in their study. This could be a reason for the discrepancies shown by this approach in SPRF. Proper usage of the efficiency function may give more accurate prediction but is not explored here.

Figure 19 compares the measured mean axial velocity along the centerline with the computed mean axial velocity, using the above mentioned three approaches. The computed data from all the approaches show the presence of the recirculation bubble in front of the center tube. The PIV data did not show this bubble, but rather shows a peak in the velocity very close to the injector. As discussed earlier, the bubble is formed due to the cylindrical cavity in the central fuel tube. It should be noted that all the computations; non-reacting premixed, reacting premixed and reacting non-premixed (will be shown later) show the recirculation bubble, while the PIV data could not. Hence, it is reasonable to assume that the PIV data might not be accurate very close to the injector. The size of this
bubble is same as that of the center tube diameter (4.1 mm) in the radial direction in both non-reacting and reacting cases. However in the streamwise direction, it is double the size of the central tube in both the cases. The main difference is that the reverse flow velocity inside the recirculation bubble for the reacting case is twice that of the non-reacting case (Figs. 15,19) as the mean axial velocity of the reacting case is also twice that of the non-reacting case. Also, note that the cavity modeled in this study is only of the size of the injector, while in the experiments, it is infinitely long.

Figure 19 shows that overall, there is a good agreement between the LES and PIV data. A peak velocity of 115 m/s occurs at \( x = 50 \text{ mm} \) due to the merging of the annular jet. This peak is reasonably well predicted by all the approaches within an error of 3 %. The PIV data, on the other hand, shows that the annular jet merges immediately after the jet enters the combustor. Hence, the peak occurs much earlier in the measurements. The velocity decay is well predicted by LEMLES when compared with the other approaches. The LEMLES prediction of the axial velocity is slightly overpredicted throughout the regions of heat release, and underpredicted very near the injector as well as at the very end of the combustor. The reason for the overprediction could be an artifact of the strong heat release rates predicted along the shear layers, as observed in Fig. 18. However, both EBULES and TFLES underpredicted the axial velocity beyond \( x = 125 \text{ mm} \). The reasons for this will be made clear in the later sections. Overall, the LEMLES results compare well with the experimental data when compared with the other approaches.

Figure 20 shows the radial profiles of the mean axial velocity at four axial locations. The velocity profiles decay downstream of the injector. The velocity profiles from all the approaches are comparable to each other and with the measured data at all the locations, except at \( x = 187 \text{ mm} \). Both the TFLES and EBULES approaches underpredicts the velocities at \( x = 187 \text{ mm} \), but the LEMLES predictions are closer to the experiments. The underpredictions are primarily attributed to the absence of heat release release near \( x = 187 \text{ mm} \) in EBULES and TFLES.

The radial profiles of the RMS axial velocity are shown in Fig. 21, which shows better
predictions with LEMLES when compared with the other approaches. The main discrepancies are observed at $x = 113$ mm. Around this region, all the models predict heat release in the shear layer. Here, the EBU model predicts a much wider shear layer zone, which led to the calculation of the highest RMS axial velocity among all the models. The TFLES approach also does not compare well with the data at this location. Only LEMLES compares well relatively at all the locations. The magnitude of the RMS values remained high even around $x = 187$ mm in all three approaches. This indicates that the heat release generates turbulence in these regions. This trend is well predicted by all the numerical approaches.

The time averaged velocity data in Figures 19, 20, 21 show that LEMLES results match well with the data. The other approaches, due to the inaccurate heat release predictions, did not compare well. However, both the TFLES and EBULES results demonstrate their capability of capturing the flow physics of the SPRF configuration with some reasonable accuracy. Even though the mean axial velocity solution looks similar, the species and the temperature field can be very different from the experiments. Next, species and temperature measurements are compared with that of the computed temperature and species from the three approaches.

Figure 22 shows the measured and the computed temperature profiles along the centerline. All three computational approaches show some discrepancies near the injector ($< 100$ mm). However, downstream, LEMLES is able to capture the trends and predictions within the error bars. Both TFLES and EBULES deviate from the experiments downstream. Also, in the case of LEMLES, the temperature predictions are saturated beyond $x = 200$ mm. No such trend is observed in the TFLES and EBULES calculations. The peak temperatures predicted in LEMLES are also the highest among all the approaches.

Figure 23 presents the CO$_2$ mole fraction profiles along the centerline. As shown, LEMLES is superior to other models in capturing the experimental data. Both experiments and LEMLES show the same saturated levels of the product mole fraction. TFLES and EBULES predictions again deviate from the experiments in the downstream region. These two approaches underpredict the products mole fraction in the stagnation region, and hence underpredict the temperature in these regions. The reason for this will be clear by looking
at the fuel mole fraction along the centerline.

Figure 24 compares fuel mole fraction along the centerline. LEMLES results show that the fuel is completely consumed at $x = 200\ mm$ whereas both TFLES and EBULES show significant amounts of $CH_4$ even beyond 250 mm. As a result of this incomplete combustion, the products produced in the TFLES and EBULES approaches are lesser in the stagnation zone leading to lower temperatures. As a result of the incomplete combustion, some amount of the fuel escapes the combustor through the reverse flow. Figure 25 shows the radial variation of the fuel mole fraction at $x = 57\ mm$. In the figure, the $x$-axis shows the radial distance. On the left is the combustor centerline, where the fuel mole fraction is the highest. Beyond the radial location of 20 mm (which corresponds to zero axial velocity contour), it can be considered to be the reverse flow jet. Clearly, LEMLES shows no traces of the fuel in the reverse flow due to the complete combustion. However, both EBULES and TFLES show considerable amounts of fuel in the reverse stream. This supports the conclusion that the fuel escapes through the reverse flow in the EBULES and TFLES approaches.

### 6.2.2 Instantaneous results

Figure 26 shows the filled contours of the instantaneous reaction rates predicted by the numerical approaches. The figure shows the first 100 mm length of the combustor. The injector is located on the top in the figure. Only half the plane in the figure is superimposed with the $z$ vorticity ($z$ is pointed out of the plane). As shown, the flame is attached to the injector lip in all the cases. The flame represented in all three approaches tends to wrap the vortical structures. The main difference to note is that the flame in LEMLES is highly wrinkled by the vortical structures when compared to the other approaches. These wrinkling effects increase the consumption area, thereby enhancing turbulent mixing and the reaction rates. LEMLES accurately captures these effects, while the EBULES and TFLES (as implemented here) approaches can not.

The lower reaction rates in the TFLES approach will also lead to higher chemical times. For the fuel oxidation reaction, chemical times are evaluated at different locations in the combustor. As an example, the chemical time in the reverse flow at $x = 100\ mm$ from the
injector is found to be 14 ms. Now, assuming the average velocity of the return flow to be 15 m/s, the fluid particle at this location takes 7 ms to flow out of the combustor. During this time, the fuel in the reverse flow can not be destroyed completely as the required chemical time is larger than the flow residence time. This is also an indication that the fuel escapes through the outflow in the combustor. The chemical time in the stagnation zone in the TFLES approach is less than 10 ms. Similar calculations are performed in the flame zone in the LEMLES approach. The chemical times are of the order of 1 ms, which is very low. As a result, there is enough time for fuel to burn completely in the LEMLES approach.

Figure 27 shows the instantaneous temperature contours in all three numerical approaches. The contours in the TFLES are more diffused due to the increased diffusivities in this model. The flame also stretches up to the stagnation end plate of the combustor. EBULES does not show any flame structure like the TFLES and LEMLES. Again, the flame surface is highly wrinkled in the LEMLES simulations.

Understanding the reasons for the discrepancies in the reaction rates in the TFLES and EBULES approaches requires analysis of the underlying assumptions behind the closures. It must be noted that small scale mixing, molecular diffusion and chemical kinetics occur at small scales and none of these processes are resolved in LES. These effects are included using the sub-grid closure models. In EBULES, the sub-grid effects are included in the computation of the reaction rate using a very simple mixing time based on the sub-grid turbulent kinetic energy. This assumption is valid only if turbulent mixing controls the combustion process. In practical combustors, various flow conditions can co-exist and hence the application of this model yields inaccurate results. In addition, the sub-grid mixing is closed using an eddy viscosity hypothesis, which is questionable due to the anisotropic nature of the species field at the sub-grid level.

In TFLES, the flame is artificially thickened by increasing the molecular diffusivities and decreasing the reaction rates. Thus, the steep gradients of the species and the temperature across the flame can be well resolved by the coarse LES mesh. Also, the chemical reaction term does not require any closure due to the thick flame assumption. However, now that the flame is thicker than the original, all the turbulent eddies smaller than the thickened flame
can not interact with the flame any more. This is the main reason why the flame predicted with the TFLES approach (Figs. 26, 27) shows less wrinkles. Also, eddies larger than the thickened flame will interact with the flame, but their interaction gets modified due to the increased flame thickness. Hence, in this approach along with the missing LES sub-grid effects, the effect of the LES resolved scales on the flame must also be corrected. These corrections are provided using the efficiency functions \( E \). As pointed out in the previous section, the appropriate functions have not been used in this study. In TFLES, the reaction rates are amplified by this efficiency function and diminished by the flame thickening factor \( F \). Hence, if \( E \) and \( F \) are not chosen properly, the computed rates will be inaccurate. The value of \( F \) in the current studies is chosen to be a function of the reaction rate. The regions with higher reaction rates will have higher flame thickness. It was observed that in the reverse flow, the appearance of reactants lead to non-zero reaction rates. As a result, the flame thickening factors higher than 1 are computed in the reverse flow. Since the reaction rates are decreased by this factor, the rates used in the conversion of species are reduced. Hence, the implemented approach does not provide enough rates for the fuel to burn in these regions. So, by accurately including a procedure to compute the rates in these regions, the model can eliminate the fuel loss and improve predictions in the premixed mode.

Contrary to EBULES and TFLES, the LEMLES approach models all of the sub-grid processes in a DNS fashion. The sub-grid diffusion, sub-grid scalar mixing, and the chemical kinetics are all resolved inside a 1D LEM domain embedded in each LES cell. Thus, LEM has a direct closure for the scalar fields. As a result, as with the velocity predictions, the scalar predictions are more accurate than the other models. This is expected from the LEMLES calculations. LEMLES solves the filtered continuity, momentum and energy equations at the LES level, but the scalar fields are explicitly evolved at the super and sub-grid levels. Proper coupling between the large scales resolved in LES and the small scales modeled by LEM enables the accurate prediction of both the velocity and the scalar fields.

The computed results show the advantages and disadvantages of each of the numerical approaches. Even though the velocity field from all three approaches showed reasonable
agreement, only LEMLES results compared well with the species and temperature measurements. Validation of the velocity results does not imply that the species and temperature fields are accurately predicted. Accurate prediction of the species and temperature fields depend on the accurate representation of the sub-grid effects.

The performance of the different combustion chemistry closures can lead to an understanding of the flame structure in the SPRF combustor. The failure of the EBULES approach to predict the flame structure indicate that in this combustor, the reactions are not completely dominated by the turbulent mixing. The kinetics also dominate the combustion phenomenon. The studies showed that a proper implementation of the model parameters can resolve the flame structure by the TFLES approach. This shows that the flame in the SPRF combustion is like a conventional premixed flame, for which the model is specifically developed. Also, the flame could be accurately predicted using the assumption of thick flames.

6.3 Reactive jet - complex kinetics

In this section, the premixed reactive case is revisited with the reaction rates closed by complex kinetics. The details of the kinetics are given in chapter 3. It was also shown earlier that the complex kinetics case (R2) is almost 33 times more expensive than the simple reduced kinetics case (R1). Hence, the simulations were run for only 2 $\tau$ and the time averaged data during this period is presented here. The primary reason for running only 2 $\tau$ is the exorbitant cost. In addition, differences between the results from the R1 and R2 simulations are very minimal. Hence, the R2 case was not run for a longer time. These issues are described below.

Comparisons of the heat release from the R1 case, the R2 case and the experiments are shown in Fig. 28. Heat release in the R2 case is computed using the expression in Eq. 85. The procedure followed to generate these plots is the same as that used in Fig. 18. The overall global features, such as the length of the flame are the same in both the R2 and R1 cases. Most of the differences are seen close to the injector. The R1 case predicted very high heat release near the injector, whereas it is very low for the R2 case. This could be
attributed to the presence of highly diffusive radicals in the R2 case. This will be more clear by looking at the instantaneous reaction rates of different species. Figures 29, 30, 31 show the reaction rates of the fuel, CO and CO$_2$ respectively in the R1 and R2 cases. The reaction rates in the R2 case are higher than that in the R1 case. Also, the reactions in the R2 case occur in the thinner regions than the R1 case. The major differences between R1 and R2 are observed in the CO$_2$ reaction rates. Clearly, CO$_2$ begins to form very close to the injector in the R1 case, whereas the formation of CO$_2$ is delayed in the R2 case. Most of the heat release is usually associated with the formation of CO$_2$. The CO$_2$ reactions in the R2 case occur further downstream than the R1 case. Hence, this is also reflected in the average heat release. Figure 28 also shows that the heat release in R2 occur in a more compact manner than the R1 case. This could be due to the thinner reaction zones in the R2 case. Even though the R2 case shows an absence of heat release very near the injector, it still shows some heat release in the first quarter of the combustor, however experiments do not detect any chemiluminescence signal (Instantaneously, heat release is observed near the injector.). The simulation uses adiabatic wall conditions because of which the walls of the injector are very hot. Some heat losses can be expected in the experiment which can cause lower reaction rates near the injector. These issues have not been explored in the computations.

Figure 32 shows the instantaneous and mean contours of the OH mass fraction. OH is highest inside the flame front and reaches an equilibrium value of 0.0003 away from the flame. Figure 32 also shows the comparison of the time averaged OH mole fraction with the processed OH PLIF data. The processed data is obtained by tracking the high OH gradient contours at each instant and averaging these contours over a number of time frames. Both experiments and computations show dark regions near the injector along the centerline. These regions represent pure reactants in the mean sense. Along with the unburnt reactants, products are also present in these dark regions (presence of the products will be shown later). The products mix with the reactants, increasing the reactivity of the mixture. Both computations and experiments show that the location at which reactions occur is about 120 mm away from the injector. The width of the reactant core is very well
predicted.

Figure 33 compares the mean axial velocity along the centerline in both the R1 and R2 cases. The R2 case shows higher velocities than the R1 case in most locations, but overall, the predictions of R2 follow the R1 predictions. Figure 34 shows the radial profiles of the mean axial velocity at four axial locations. The predictions of R2 are identical to the predictions of the R1 case. Discrepancies are mainly observed in the centerline data at 113 and 187 mm from the injector. Figure 35 compares the radial profiles of the RMS of the axial velocity at four axial locations. The predictions of the R2 case matches more closely with the experiments. In particular the near field predictions are very accurate in the R2 case. Further downstream, the R2 case shows some differences with the measurements. Other than the near field, the predictions of the R1 and R2 cases are almost similar.

Figures 33, 34, 35 show that the velocity field predictions in both the R1 and R2 cases are identical. The main differences are observed in the flame structure in the near field. The R1 case shows higher heat release very near to the injector whereas the R2 case shows little or no heat release near the injector. The predictions of the heat release near the injector in the R2 case is in agreement with the experiments. This could be the reason for the good predictions of the RMS axial velocity near to the injector in the R2 case.
Figure 15: Comparison of the centerline mean axial velocity for the non-reactive jet.

Figure 16: Comparison of the radial profiles of the mean axial velocity for the non-reactive jet.
Figure 17: Comparison of the radial profiles of the RMS axial velocity for the non-reactive jet.

Figure 18: Comparison of averaged heat release rates along a plane passing through the centerline for the reactive jet. The units of heat release in the computations is Joule/sec.
Figure 19: Comparison of the centerline mean axial velocity for the reactive jet.

Figure 20: Comparison of the radial profiles of the mean axial velocity for the reactive jet.
Figure 21: Comparison of the radial profiles of the RMS axial velocity for the reactive jet.

Figure 22: Comparison of the centerline variation of the temperature. Units of temperature is $K$. 
**Figure 23:** Comparison of the centerline variation of the $CO_2$ mole fraction.

**Figure 24:** Comparison of the centerline variation of the fuel mole fraction.
Figure 25: Comparison of the radial variation of the fuel mole fraction.

Figure 26: Instantaneous fuel destruction reaction rate contours with the superimposed vorticity contour lines on one half of the plane.
Figure 27: Contours of the instantaneous temperature (K).
Figure 28: Heat release predictions from LEMLES with simple kinetics (R1) and LEMLES with complex kinetics (R2). Units of the heat release in computations is J/s.
Figure 29: Contours of the fuel destruction rate. Units of the rate is $kmol/m^3s$. 

92
Figure 30: Contours of the CO reaction rate. Units of the rate is \( Kmol/m^3s \).
Figure 31: Contours of the $CO_2$ reaction rate. Units of the rate is $Kmol/m^3s$. 
Figure 32: Contours of the mean and instantaneous $OH$ mass fraction.
Figure 33: Comparison of the centerline mean axial velocity.

Figure 34: Comparison of the radial profiles of the mean axial velocity.
Figure 35: Comparison of the radial profiles of the RMS of axial velocity.
CHAPTER VII

COMBUSTION AND FLOW CHARACTERISTICS IN
THE PREMIXED CASE

This chapter addresses the flow features in both the non-reacting and reacting cases in the premixed mode. The combustion characteristics such as the flame structure and emissions are also discussed.

7.1 Flow features

Figure 36 shows an instantaneous snap shot of the pressure contour field in the non-reacting case. The contours are shown along a plane passing through the centerline. The injector is located at the top and the flow is from the top to the bottom. For the sake of better visualization, only the first 100 mm length of the combustor is shown in Fig. 36. Pressure structures seem to be shed from the annular injector and they propagate along the shear layer. The size of the large scale structures increases in the streamwise direction up to $x = 90$ mm. This is around the region where the shear layers merge. Beyond this location, the coherent structures are partly dispersed and after 100 mm, they are completely dispersed. The shedding of the structures can also be identified by plotting the instantaneous pressure fluctuations. Figure 37 shows the contours of the instantaneous pressure fluctuations in the non-reacting case. The plot is generated by subtracting the mean pressure from the instantaneous pressure. The roll up of the vortices in the outer shear layer of the annular jet are clearly visible in the figure. The size of the vortices increases up to $x = 50$ mm and then decreases further downstream. The vortices are also observed to pair up as their size increases and then they break up and diffuse. This is due to vortex stretching and viscous effects.

The 3D nature of the instantaneous flow field can be visualized using instantaneous velocity contours. Figure 38 shows the instantaneous axial velocity contours on a 2D radial
plane that cuts at different axial locations at two different instants, for both the non-reacting and reacting cases. In the non-reacting case, the time difference between the two instants is 0.5 ms, while in the reacting case, it is 0.25 ms. The injector is located at the top and the flow is from the top to the bottom. The non-reacting jet stagnates as early as 200 mm from the injector. At both instants, the cold flow jet maintains a core-like structure until the middle of the combustor. As the jet exits the injector, the core first expands and then diminishes when it reaches the 2/3rd length of the combustor. In the reacting case, the inflow velocity is almost twice that of the non-reacting case, due to the preheating effect discussed in chapter 4. Hence the velocity scaling is doubled for visualization in the reacting case. The reacting jet reaches all the way to the stagnation end plate. Similar to the non-reacting case, the jet core first expands outside the injector, but here the core size gets bigger than that in the non-reacting case. The reacting jet no longer maintains the simple jet-like structure in the middle of the combustor. The core randomly moves around the center and starts to break up at $x = 100$ mm. This is the region around which significant heat release occurs. Heat release causes the jet to expand and hence pushes the jet in all directions. The axial expansion causes the jet velocity to remain non-zero till the stagnation end plate. The radial expansion causes the jet to expand radially so that the jet core expands in the radial direction. The tangential expansion causes the jet to expand laterally which causes lateral motion of the jet. The lateral movement of the jet is more evident in the reacting case than the non-reacting case at the two instants shown in Fig. 38. The expansion also decreases the effective area of the return flow stream, which leads to an increase in the return flow velocity.

Figure 39 shows the instantaneous axial vorticity contours for both the cases. For the non-reacting case, vorticity is at its highest in the shear layer near the injector. It gradually dissipates and finally reduces to nearly zero midway through the combustor. For the reacting flow, however, the axial vorticity increases in the downstream direction extending up to as much as 100 mm away from the injector. The increase in the vorticity is likely due to the generation of baroclinic torque, which is a result of the heat release/expansion processes in this part of the combustor. Hence, there is flame generated vorticity (FGV). Although, the
magnitude of vorticity is reduced away from the heat release zone, it persists almost all the way down to the stagnation end of the combustor.

To quantify the FGV phenomenon within the combustor, and to provide additional insight into the vorticity, different terms of the vorticity transport equation are going to be examined.

\[
\frac{\partial \omega}{\partial t} + \vec{u} \cdot \nabla \vec{w} = (\vec{w} \cdot \nabla)\vec{u} + \nu \nabla^2 \vec{w} - \vec{w}(\nabla \vec{u}) + \frac{1}{\rho^2} (\nabla \rho \times \nabla P) \tag{86}
\]

where \(\vec{u}, \vec{w}, \rho, \) and \(P\) are the velocity vector, vorticity vector, density and pressure respectively. The equation has the vorticity convection term on the left side and the vortex stretching term, the viscous diffusion term, the dilatation term and the baroclinic torques terms on the right hand side (shown in order in equation 86). Terms that redistribute vorticity, such as convective terms, do not change the total vorticity and thus do not contribute to FGV. Only two terms in the vorticity equation can create vorticity where none was originally present before; these are the viscous term and the baroclinic torque term. The stretch term cannot create new vorticity, but can amplify or attenuate the total vorticity. The creation of vorticity by a flame is entirely due to the baroclinic torque term \([62]\), and this has been studied in detail in the literature\([96, 67]\). The term creates vorticity across the flame by the misalignment of the density gradient and the pressure gradient. Since, the density gradient across the flame is very large, any small misalignment of the gradients may produce significant FGV. Figure 40 shows the instantaneous visualization of the baroclinic torque in the \(z\)-direction (perpendicular to the plane). Both positive and negative regions can be observed close to the flame surface. Thus the baroclinic torque component either suppresses or creates the vorticity. Since the flame is highly wrinkled, sign changes occur very frequently. The baroclinic torque is present only along the the flame front.

It should be noted that the baroclinic torque plays a significant role only in the reacting cases and thus the increased levels of vorticity in the reacting case is primarily due to this term.


7.2 Flow scales

It is of interest to compute the sizes of the large and the small scale eddies and the range of eddies present in the flow. The large scale structures will be responsible for the mixing characteristics in the combustor. LES has the ability to accurately capture these large scale structures. The large scales represent the characteristic energy-containing eddies that play a major role in the transport of energy and scalars. The size of the large scales is computed in the axial direction using the definition of longitudinal integral length scale.

\[
R_L(r) = \frac{\overline{\Delta u(x) \Delta u(x + r)}}{u'(x) \cdot u'(x + r)}, \quad L_T = \int_0^\infty R_L(r)dr \Delta u = u - \overline{U}
\]  

(87)

Here, \( R_L \) is the correlation coefficient, \( u \) is the instantaneous axial velocity, \( \overline{U} \) is the mean axial velocity, \( u' \) is the RMS of axial velocity and \( L_T \) is the integral length scale. The above expression is used with a modification in the current studies. All the quantities \( (u, \overline{U}, u') \) in the above equation are replaced with the LES resolved variables, which is expected to provide an estimate of the LES resolved large scale structures. The estimated scales are shown in Fig. 41. The figure shows the variation of the size of the large eddies along the axial direction at radii of 2 and 9 mm. The size of the large scale structures increases up to \( x = 100 \text{ mm} \) and then remain constant from 110 mm to 180 mm. After this location, the eddy size reaches its maximum value, after which it decreases due to the confinement caused by the walls in the stagnation region. The size of the eddies are found to increase away from the centerline (2 mm to 9 mm). Thus, the size of the large scale eddies in the returning flow is larger than those in the forward motion jet.

In order to determine the range of turbulent scales in the SPRF combustor, the size of the Kolmogorov eddies in the shear layer are computed using the sub-grid Reynolds number. The smallest Kolmogorov eddy in the domain is 0.06 mm, whereas the size of the LES resolved large eddies is 6 mm. Hence, the range of turbulent scales found in SPRF are two-order-of-magnitude (O(2)).
7.3 Jet entrainment

Entrainment effects are studied in both the non-reacting and reacting cases. The jet entrainment is computed using the conventional definitions of the jet mass flux at different cross sections in the axial direction. In this work, the entrainment rate based on the mass flow rate is used and is given by \( e = \dot{m}_e/\dot{m}_o \), where \( \dot{m}_e = \int_0^R 2\rho u r dr \). Here, \( \dot{m}_o \) is the inflow flow rate and \( R \) is radius at which the axial velocity \( u \) is zero. Figure 42 shows the computed jet entrainment. Both non-reacting and reacting jets attain maximum entrainment levels and then decrease due to the decay of the axial velocity of the jet. A steep initial increase in the entrainment levels is shown by both the non-reacting and reacting jets. This is mainly due to the confinement of the combustor [60]. Note that the entrainment reaches a maximum at \( x = 90 \) and 65 mm in the non-reacting and reacting cases, respectively. The reacting jet maintains a non-zero mass flow rate up to an axial distance of \( x = 250 \) mm due to the non-zero axial jet velocity. The maximum entrained mass in the cold flow is about 2.6 times larger than that calculated for the reacting case. Han and Mungal [38] showed that for a jet flame, the entrainment reduces by a factor of \((T_b/T_u)^{0.5}\) due to heat release. This factor is equal to 1.95 in the current studies.

The entrainment in the SPRF combustor is analyzed with that in a momentum driven free jet. The main difference is that the entrainment in a free jet keeps increasing with the axial distance, but this will not the case in the SPRF combustor. Hill [40] measured the local entrainment rates in a free jet and obtained a simple expression as, \( e = C_e x/d^* \) where, \( d^* \) is equivalent source diameter and \( C_e = \frac{d^*}{m_0} \frac{dn}{dx} \). Using this expression and assuming that virtual origin corresponds to \( x = 0 \) with \( d^* \) as the inner diameter of the annular tube, \( C_e \) is evaluated in both non-reacting and reacting cases in the SPRF setup. The variation of the entrainment coefficient \( C_e \) along the axial distance is shown in Fig. 43. The coefficient \( C_e \) first increases and then decreases in both the cases. The maximum value of entrainment coefficient in the non-reacting case is 0.32 and this is reached at 53 mm (3.5 jet diameters) from the injector. Hill [40] showed that this coefficient reached 0.32 in a free jet at about 13 jet diameters. This gives an indication that the entrainment levels in the SPRF combustor are higher than that of a free jet. In the reacting case, \( C_e \) reaches a maximum value of 0.24
at 7 mm from the injector and then decreases. Han and Mungal [38] reported 0.13 for a momentum driven reacting jet.

Figure 44 shows the zero contour of the mean v velocity in x-y plane for both the cases. In the figure, red color denotes the positive y-velocity (going right) and blue color denotes the negative y-velocity (going left). Also, the zero mean axial velocity contour is marked in black. In the figure, the intersection point of the zero axial velocity contour and the zero v velocity contour is marked as A. The location of this point A in both the cases match with the location of the maximum entrainment (refer Fig. 42). This implies that it is the v velocity component which determines the rate of increase of entrainment [2]. In addition, along the zero axial velocity vector, the v velocity is pointed towards the centerline upstream of point A and it is pointed away from the centerline downstream of point A. This shows that upstream of point A, the v velocity directed towards the jet causes entrainment of the return flow. Downstream of point A, the v velocity is directed away from the jet because of which the jet entrainment is absent. This is the main reason for the peak mass entrainment at point A in both the non-reacting and reacting cases. Another interesting observation is that, along the zero axial velocity contour, the v velocity is highest close to the injector and then decreases downstream. To show this quantitatively, the radial profiles of the mean v velocity at x = 75 and 25 mm are shown in Fig. 45. Both the reacting and non-reacting cases show higher v component at x = 25 mm. Most importantly, the v velocity is higher at the location where the axial velocity is zero. Hence, the entrainment is highest close to the injector and then decreases downstream. The higher velocity of the v component very near to the injector is primarily due to the higher pressure gradients that drive the flow radially into the jet. These gradients are created by the merging of the high momentum annular jet and they decrease once the jet merges. The v velocities in the reacting cases are higher than the non-reacting, which suggests higher entrainment, but Fig. 42 shows a lower mass entrainment for the reacting case compared to the non-reacting case. This is most likely due to the low density of the products that are being entrained in the reacting case.

Figure 46 shows the entrainment predicted in the R2 case. The entrainment levels in the R1 and R2 cases are similar in the near field. Both cases attain peak values at approximately
$x = 65\ mm$. After this point, the entrainment in R2 shows higher values than the R1 case. Since no mass can flow into the forward jet after 65 mm from the injector, the increased levels are attributed to the slightly higher mean velocity predicted in the R2 case. The reason for the similar entrainment in R1 and R2 can be explained using the radial profiles of the mean $v$ velocity. Figure 47 compares the radial profiles for R1 and R2 cases at $x = 10, 20$ and $40\ mm$. At all three locations, the magnitudes of $v$ velocity components are nearly identical. Hence, the mass entrained in the near field is identical in both the cases.

The above discussion shows the importance of the 3D nature of the flow. Mean radial and tangential velocities for both the non-reacting and reacting cases at different axial locations are shown in Fig. 48. The magnitudes of radial and tangential velocities are very small when compared to the axial velocity component in both the cases. It should be noted that the reacting case shows higher radial and tangential velocities. The variation of the RMS of the radial and tangential velocities at different axial locations for both the non-reacting and reacting cases is plotted in Fig. 49. It is interesting to see that the magnitudes of both velocity components are identical throughout the combustor in the non-reacting case. The RMS values attain similar values as that of the axial component at $x = 245\ mm$ in the non-reacting case. For the reacting jet, $v_{rms}$ magnitude is much higher than the $w_{rms}$ at $x = 57\ mm$, but downstream, the profiles become comparable, $120\ mm$ from the injector. In the non-reacting case, all the three components are comparable after $x = 200\ mm$ from the injector, whereas in the reacting case, the components are comparable as early as $100\ mm$ from the injector. In the non-reacting case, beyond $187\ mm$ from the injector, the mean components are smaller than the RMS components. Similar regions are also present in the reacting case but only beyond $x = 240\ mm$ [35]. Both $v$ and $w$ components of the reacting jet are higher than that in the non-reacting jet throughout the combustor.

### 7.4 Turbulence production

The effect of heat release on turbulence is analyzed here. The current computations use a sub-grid turbulent kinetic energy equation Eq. 23 to model the interaction of large and sub-grid scales. The production term in this equation gives the rate at which energy is
transferred through the cascade from large to small scales. This production term within
the combustor for both non-reacting and reacting cases is shown in Figure 50. Turbulence
production levels are high near the injector in both cases due to the strong shear layers.
Turbulence production is also high inside the recirculation bubble, which is located in front
of the central tube. The main difference between the non-reacting and the reacting case
is the center part of the combustor. In this region, turbulence production is higher in the
reacting case. These regions coincide with the heat release regions. Heat release causes
volume expansion, which accelerates the flow and increases kinetic energy of the fluid. This
energy is transferred to the small scales through the non-linear action of the eddies on
the mean velocity gradients. The rate at which these interactions occur increases with the
energy present. Thus, the higher energy due to heat release leads to higher turbulence
production than that in the non-reacting case. Along with the production, the dissipation
contours are also shown at the same instant. It can be observed that production and
dissipation are of similar magnitude throughout the combustor in the non-reacting case,
which shows that there is an equilibrium between production and dissipation. However,
in the reacting case, differences between production and dissipation are observed in the
heat release regions, which shows that heat release can cause non-equilibrium effects in the
turbulence kinetic energy balance.

7.5 Product entrainment

In the SPRF combustor, there is no external preheating. The exhaust gases during their
return path mix with the incoming reactant mixture and provide internal preheating effects.
The dynamics of this phenomenon are demonstrated here. Firstly, preheating of reactants
along the centerline is presented. Figure 51(a) shows the variation of different parameters
across the flame at 3.6 Dia from the injector. This location is chosen in such a way that the
flame at this location never crosses the center-line at all instants of time. This statement is
supported using the scatter plot shown in Fig. 51(b). The plot shows the fuel destruction
rate along the center-line at different time instants and it is evident that the reaction rate
is absent at 3.6 Dia from the injector. This supports the claim that the flame surface never
crosses the center-line at this location. This location is chosen in Fig. 51(a) so that it is possible to demonstrate the preheating effects isolated from other effects. In the figure, the location of the flame is marked by the the non-zero reaction rate. The left side of the flame with the pure reactants is the reactant side and the right side with the pure products is the product side. Figure 51(a) shows that on the reactant side, the products are present. These products can be seen along the centerline if the instantaneous flame crosses the centerline. However, Fig. 51(b) shows that flame never crosses the center-line at this location. Thus, the products entered into the reactant stream through a different mechanism (will be explained later) in the SPRF setup. Also, the temperature variation across the flame is shown in Fig. 51(a). The temperature begins to increase even before the reactions occurred showing the preheating effects due to the presence of products. The temperature further increases across the flame due to the reactions. Hence the temperature rise across the flame happens in two stages, first rise is through the preheating and the second rise is through the reactions. Figure 51(a) indicates internal preheating due to the presence of products inside the flame. It is yet to be understood how these products are penetrating into the reactant stream.

The velocity vectors along with the isocontours of the reaction rates near the combustor region are shown in Fig. 52. Also, the velocity vectors are colored by the products mass fraction. The plot shows that the velocity vectors carrying the products are pointing into the flame surface at some locations. These vectors can penetrate into the reactants side only if the flame is either broken or the reaction rates are extremely low. Figure 52 shows that there are broken reaction zones on the flame surface and it is through these broken zones (or holes) that the velocity vectors carrying the products are penetrated into the reactant stream. These broken zones exist along the shear layer between the forward flowing reactants and the reverse flowing products and the flame is extinguished in these regions. This feature of product penetration is termed as "product entrainment" [11], which is different from conventional jet entrainment. Experiments are also performed to demonstrate this product entrainment. Raman Spectroscopy was used to measure the species mole fraction. However, because of the limitations of the measurement technique [11], the data
is measured only up to 13 Dia (one Dia = 12.5 mm) from the injector. The product gases mole fraction from experiments and LEMLES are plotted along the center-line in Fig. 53. This figure further establishes the fact that products are present along the center-line in both the computations and experiments. Their presence is seen even at 3 Dia from the injector. The over-all agreement in Fig. 53 is very good. The products mole fraction reach saturated levels at about 18 Dia in the combustor. This is an indication of the length of the flame in a mean sense. However, the product entrainment levels are underpredicted by the computations. The reason can be traced back to the heat release predictions by the computations. LEMLES predicted stronger flame zones with higher reaction rates, than the measurements, near the injector. As a result, even though the products are entrained through the local broken flame zones, because of higher reaction rates, the entrainment could be underpredicted. In other words, a strong flame will not let products go through when compared to a very weak flame. Hence, the entrainment levels could be underpredicted in the computations. Another reason could be that the computations are underpredicting the \( v \) velocity, which was shown to be responsible for the mass entrainment. However, no measurements are available to verify the above two claims.

In the earlier discussion, the products are shown to penetrate through the broken reaction zones. However, through these broken zones, not only can products enter into the reactant stream, but the reactants can go outside the flame. In order to find this, radial profiles of the mean \( CO_2 \) and \( CH_4 \) are plotted at different axial locations near the injector. The profiles, together with the mean flame locations is given in Fig. 54. The figure shows that products are present inside the flame but the reactant do not show up beyond the flame location. Hence, in the SPRF setup, only the products are able to enter into the reactant stream while the reactants do not escape out of the flame. These products are entrained into the flow by the vortical structures present in the reverse flow products.

### 7.6 Flame structure

The SPRF premixed flame represented by the fuel destruction reaction rate is shown in Fig. 55. The flame is highly convoluted due to the action of turbulent structures and extends
up to the second half of the combustor. Pockets of unburnt reactants are separated from the flame and burn completely downstream. The rest of this section provides a detailed analysis of its flame structure.

In order to determine different combustion regimes and understand the turbulent flame structure in the SPRF combustor, a Borghi diagram [13] modified by Pitsch [84] for LES applications is used. The analysis requires total RMS velocity \( v'_{\Delta} \), LES filter size \( \Delta \), laminar flame thickness \( l_f \), and laminar flame speed \( s_l \). The RMS velocity and the LES filter width (same as grid size) can be evaluated using the data obtained from the simulations. However, the laminar flame speed and the flame thickness can only be estimated using the premixed laminar flame simulations. In the SPRF combustor, because of the internal preheating, the laminar flame speed and the flame thickness will depend on the amount of products present at that location. Hence, a parameter called product fraction \( (f_p) \) is defined to quantify the recirculation of products. It is defined as the ratio of the mass of the products to the mass of the reactants. The contours of \( f_p \) along a center-line plane are shown in Fig. 56(a). A zero value of \( f_p \) corresponds to the region where there are no products and a value of \( \infty \) corresponds to a region with pure products. Depending on the the value of \( f_p \) i.e., the amount of products entrained, different flame speeds and flame thickness can be obtained using the CHEMKIN PREMIX package. Using the flame speed and the flame thickness, Karlovitz number \( (K\alpha) \) defined for LES [84] is evaluated. A value of \( K\alpha \) less than 100 (but greater than 1) is considered to be in thin reaction zone regime [84]. In this regime, the flame is thick but the reaction zone is still thin. A value of \( K\alpha \) greater than 100 is considered to be a broken reaction zone, where the Kolmogorov size eddies are small enough to penetrate the inner layer of the flame and alter the laminar flame structure. In the SPRF combustor, for the range of \( f_p \) (refer Fig. 56(a)) found in the computations, \( K\alpha \) is evaluated. This can be visualized in Fig. 56(b), which shows the isocontours of reaction rates colored by the Karlovitz number. Since, different \( f_p \) values are found in the combustor, for the purpose of visualization, \( K\alpha \) is evaluated at a value of \( f_p = 0.1 \). The color blue in Fig. 56(b) denote the values of \( K\alpha \) less than 100 and the color red denote the values of \( K\alpha \) greater than 100. Clearly, most of the combustion occurs
in the thin reaction zones with the exception of few isolated points in the broken reaction zone. It should be understood that the above $Ka$ values are based on $f_p = 0.1$. A lower value than this corresponds to a low amount of product entrainment which occurs closer to the injector. Hence, $Ka$ evaluated based on low $f_p$ values will show more broken reaction zones near the injector. In order to further explore the regimes, few locations with different $f_p$ values are chosen from Fig. 56(a) and the values of $Ka$ are evaluated. These locations are marked on the turbulent premixed combustion regime diagram [84] shown in Fig. 56(c). Point 1 corresponds to the lowest amount of product entrainment and point 2 corresponds to the highest amount of product entrainment. The figure shows that as $f_p$ increases, the combustion regime is shifted towards the thin reaction zones. These observations can also be understood by looking at the turbulence and the entrainment characteristics along the flame location. Near the injector, the turbulence intensities are very high ($u'$) and since the preheating effect due to product entrainment is low here ($S_L$), hence if any reactions occur, it will be likely with broken zones. In the downstream region, decreasing turbulent intensities and increasing flame speeds (due to high preheating effects) will push the reactions into the thin reaction zones. Also, the heat release rates are highest in the regions that are close to the laminar flamelet regimes due to the presence of high amount of products. It should be noted that product entrainment has opposing effects on the flame speeds. Product entrainment increases preheating, that increases flame speeds but at the same time increases dilution that can reduce the flame speed. However, Bobba et al. [11] showed that the product entrainment increases the reactivity more than the reduction in the reactivity due to dilution.

The broken zones are observed on the surface of the SPRF flame. These are the regions with negligible reaction rates. Figure 57 shows the temporal and spatial evolution of $CO_2$ formation rate at different cross sections. The cross sections shown are at $x = 15$, 35 and 125 $mm$. The reaction rates represent the surface of the flame. At all the instants shown in figure, the flame is more broken at $x = 15$ $mm$ when compared to the other two locations. At $x = 125$ $mm$, the reaction rates show a well defined flame structure. Thus, the figure reveals that there are more broken or extinction regions close to the injector and
these regions decreases downstream. Hence, the products are more likely to penetrate into
the reactant in the upstream portion of the combustor when compared to the downstream
region. With time, the locations of the local extinction zones changes in the upstream
portion of the combustor. This could be most likely due to the unsteady nature of the flow
in these regions. The unsteadiness is causing the broken flames to be present at one instant
and disappear at the next instant. This situation is different from the classic situation of a
flame front oscillating around a mean location.

Flame extinction can occur due to multiple reasons. The presence of injector walls
implies heat losses from the surrounding flow and inhibition of the reaction rates due to
radical recombination. These effects are not included in the numerical simulation. However,
the quenching effects observed in the simulations can be explained based on the high velocity
gradients occurring in the shear layers near the injector. This analysis is provided by Law
[56] which shows that the stretch has two components, one from the strain rate and the
other from the curvature effects. The stretch can affect the normal mass flux entering
the reaction zone and the residence time, thus affecting the reaction rates of the chemical
reactions. The stretch effects in the SPRF combustor are studied by considering the strain
rates and neglecting the curvature effects. The strain rate is computed using the following
expression.

\[
S = \sqrt{\left[ (\frac{\partial u}{\partial x})^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] + 0.5\left[ \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)^2 + \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 \right]} \tag{88}
\]

Figure 58 shows the strain rate contours plotted over the reaction rates along a centerline
plane. The first 100 mm of the combustor alone is shown in the figure. Also, only half of the
plane is shown here. The figure shows an expected pattern of the reaction rates being very
small in magnitude in regions of high strain. And that the flame is attached to the injector
in the regions of low strain on the products side. In order to determine the threshold values
at which burning occurs, scatter plots are used here. Figure 59 shows the scatter plots of
reaction rates and the strain rates at different axial locations. At all locations, more than
99 % of the reaction rates are observed at strain rates lower than 100,000 /s. The reactions
also occur close to the injector at strain rates more than the 100,000 /s. However, the rates are an order of magnitude lower than the reaction rates in the downstream. Moving downstream, the strain rates are lower and a wider flame region with higher reaction rates is observed.

### 7.7 Emissions

The reacting studies are performed at $\phi = 0.58$, with a preheating temperature of 500 K. Also, all the walls are adiabatic in the simulations. The corresponding adiabatic flame temperature for these conditions is 1780 K, while the computed post flame temperature in the simulations is between 1850-1900 K. One of the reasons for this difference could be the simple kinetics employed in the calculations. Figure 60 shows the comparison of the temperature along the centerline. The measured temperature is from Raman technique [11]. There are discrepancies between the data at low temperatures due to the underpredicted product entrainment in the near field. The predictions in the downstream region are within the error bars. Overall the trend is well predicted. From the emissions point of view, the predicted temperature plays a critical role. Thermal $NO_x$ is primarily a function of the temperature and the residence time ($\tau$). Higher $\tau$ produces higher thermal $NO_x$. In the SPRF combustor, the value of $\tau$ computed using the definition in section 3 is around 8 ms. The simulations are run for $4 \tau$ and during this time, a global thermal mechanism [78] is used to compute the thermal $NO_x$. The simulations predicted a peak $NO_x$ of 1.5 ppm in the high temperature region of the stagnation zone. It should be noted here that the time needed for the $NO_x$ massfraction to reach statistically stationary state is much longer than that needed for the flow and other major species massfractions. The current simulations could not be run for such long times. However, it was noticed that in an instantaneous sense, the $NO_x$ levels in the simulations reached steady state and levels observed are of the same order of magnitude as those presented in this section. The statistical steady state for $NO_x$ is defined as the state when the $NO_x$ present at the outflow reaches a statistically steady state.

$NO_x$ calculations are also done as post processor calculations. For this purpose, the
global thermal $NO_x$ mechanism proposed by Turns [116] and the time averaged concentrations and temperature from the simulations are used. These calculations also showed peak emissions around 1 ppm in the highest temperature regions for the computed residence time in the combustor.

Instantaneous $NO_x$ reaction rates in LEMLES simulations using the thermal and non-thermal global steps are shown in Figs. 62(a) and 62(b). The $NO_x$ production through non-thermal path is significant only in the flame zone, whereas the $NO_x$ production through the thermal path is significant in the regions of high temperatures. In order to distinguish between the $NO_x$ formed by both paths, statistically steady solution from LEMLES is used to compute the $NO_x$ concentration. Figure 61 shows the $NO$ formed in both the thermal and non-thermal pathways in 4 $\tau$. The plot shows that $NO_x$ formed from both paths is comparable and that the non-thermal $NO_x$ is produced inside the flame and disappears once $CO$ is destroyed. This is because the reaction rate for the non-thermal $NO_x$ is a function of $CO$ concentration. In order to further analyze the non-thermal $NO_x$ levels, PREMIX (CHEMKIN package) calculations are performed using the SPRF operating conditions. $NO_x$ levels are noted at the flame front, i.e., location at which the temperature gradient is the steepest. This represents the $NO_x$ formed by means other than thermal route and its value is found to be 2 ppm. This supports the values predicted by the computations. Thus, the above discussion shows that NOx produced by the non-thermal route is similar to that produced by the thermal route. However, at the predicted peak temperature of 1900 K, the thermal $NO_x$ will be higher than that at the adiabatic flame temperature of 1780 K. Hence, it could be possible that emissions in the SPRF are primarily from non-thermal routes.

The SPRF configuration aids in the dilution of the reactants with the products. As a result, the oxygen concentration is reduced. This trend is observed in Fig. 61. The oxygen mole fraction reaches low levels in the heat release zone, where combustion occurs. Also, in the stagnation zone where thermal $NO_x$ can be higher than the other locations, the $O_2$ mole fraction is the lowest. It is well known that the presence of lower oxygen content in the flame envelope and in the combustion products reduces $NO_x$. This is also a reason for low $NO_x$ emissions in SPRF. As an illustration, thermal $NO_x$ emissions are
proportional to the square root of the oxygen concentration [116]. So, by reducing the oxygen content in the combustion air from 21 to 16% will reduce emissions by approximately half. This lower oxygen concentration can also lead to lower CO emissions. The simulations employed a reduced as well as a detailed kinetic model for CO kinetics. The predictions from both simulations are highest inside the flame. The simple kinetics (R1) predicted almost negligible CO in the post flame zone and near the outflow, but the detailed kinetics (R2) predicted values around 30 ppm in the post flame zone and about 15 ppm near the flow. This is in very good agreement with the experiments which observed around 12 ppm at the outflow. Thus SPRF exhibits very low CO and NO\textsubscript{x} emissions in the premixed mode of operation. Low oxygen content along with low temperature lead to such low emissions. In addition, the internal preheating demonstrated in the computations is stabilizing the flame even at low equivalence ratios. Thus, very lean conditions can be attained in the combustor leading to ultra low emissions.
Figure 36: Instantaneous pressure contours in the non-reacting case. Units in Pascals.
Figure 37: Contours of the instantaneous pressure fluctuations in the non-reacting case. 
Units in Pascals.
Figure 38: Instantaneous contours of the 3D axial velocity.
Figure 39: Instantaneous contours of the 3D axial vorticity.
Figure 40: Instantaneous contours of the z-direction baroclinic torque. Units in $1/s^2$
Figure 41: Centerline variation of the size of large scale eddies in the axial direction

Figure 42: Entrainment rates
Figure 43: Variation of the entrainment coefficient

Figure 44: Contours of the zero $v$ velocity and zero axial velocity. The boundary between the blue and red colors is the zero $v$ velocity contour. The dark black line is the zero axial velocity contour. The axial distance is provided in $mm$. 
Figure 45: Radial profiles of the mean $v$ velocity
Figure 46: Entrainment rates

Figure 47: comparison of the radial profiles of the mean $v$ velocity in the R1 and R2 cases
Figure 48: Radial profiles of the mean of radial and tangential velocities
Figure 49: Radial profiles of the RMS of $v$ and $w$ velocities
Figure 50: Contours of production and dissipation of the turbulent kinetic energy. Units used is $Kg/m s^3$. 
(a) Variation of different parameters across flame at $x = 45\,mm$ from the injector. Units of fuel rate and $CO_2$ rate is $kmol/m^3s$. The products are presented as mass-fraction and temperature in $K$.

(b) Scatter plot of fuel destruction rate along the centerline. Units used for rate is $Kg/m^3s$.

Figure 51: Demonstration of the preheating effects in the SPRF combustor
Figure 52: Visualization of flame in the near field showing the product entrainment. Iso-
surface of fuel destruction rate with a value of $1 \times 10^{-4} \text{Kmol/m}^3\text{s}$ is shown to represent
flame surface. The velocity vectors coloured with product massfraction ($CO_2$) are shown
along a plane passing through centerline
Figure 53: Comparison of the species mole fraction along the centerline
Figure 54: Radial profiles of the mass fraction of the fuel and air at x=60 mm

Figure 55: Instantaneous contours of the fuel destruction rate (Kmol/m³s)
(a) Mean contours of the $f_p$ defined as the amount of products to reactants. Points 1, 2, 3 and 4 denote locations with different $f_p$ values.

(b) Instantaneous isocontours of fuel destruction rate ($-1 \times 10^{-4} \text{ Kmol/m}^3\text{s}$) colored by Karlovitz number. Color blue indicates $Ka < 100$ and color red indicates $Ka > 100$.

(c) Turbulent premixed combustion regime diagram. Points shown with different $f_p$ values.

**Figure 56:** Operating mode of the SPRF combustor
Figure 57: Contours of instantaneous rates at different instants and different axial locations. Units in $Kmol/m^3$
Figure 58: Instantaneous strain rate filled contours with contour lines of $CO_2$ formation rate ($Kmol/m^3$). The blue denotes the regions with strain rates less than 100,000 /s and the red color region denotes the regions with strain rates more than 100,000 /s.

Figure 59: Scatter plots of $CO_2$ formation rate vs. strain rate at different axial locations. Units of $CO_2$ formation rate is $Kmol/m^3$s and that of strain rate is 1/s.
Figure 60: Comparison of the centerline variation of the temperature (K)

Figure 61: NO from the thermal and non-thermal pathways and the mean mole fractions of CO and O$_2$. 
(a) Instantaneous contours of the non-thermal NO production rate

(b) Instantaneous contours of the thermal NO production rate

Figure 62: Instantaneous contours of NO reaction rates. Units in $Kmol/m^3s$
CHAPTER VIII

NON-PREMIXED COMBUSTION

This chapter focuses on the non-premixed combustion in the SPRF combustor. Earlier studies [117] showed that LEMLES is the only combustion model that captures flame structure accurately in the non-premixed mode. The same approach is also used in the current studies. This chapter mainly addresses the similarities and differences between the premixed and non-premixed modes of operation and analyzes the flame structure in the non-premixed mode.

8.1 Recirculation bubble

A discussion on the onset of recirculation bubble in the co-axial jet injectors is provided in chapter 2. This section addresses these aspects in the SPRF configuration. The injector configuration is similar to that of free coaxial jets. Hence, as shown by Villermaux [118], there can exist situations (inflow boundary conditions and geometry setup) where there will be a recirculation bubble in front of the fuel jet. The parameters that are studied in the literature that may effect these near field predictions are (1) momentum flux ratio between outer and inner jet (MR), (2) confinement, (3) annular gap width, (4) inflow velocity profile at the inner jet, (5) inflow turbulence profiles and (5) retraction of inner injector with respect to the outer injector [92, 93]. During the course of the present efforts, the effect of momentum flux ratio (\(\rho_a u_a^2/\rho_f u_f^2\) where a-air and f-fuel) is found to have a dominant effect on the near field predictions.

The effect of momentum flux ratio is demonstrated here using results from two cases with different momentum flux ratios. In one of the cases, the momentum ratio is 9.9 and in the other case is 8.7. These cases will be referred to as RB and NRB, respectively. The predictions of the mean axial velocity near the injector in both cases is shown in Figure 63. The RB case clearly shows a recirculation bubble with negative velocities as high as 20
m/s, where as this is absent in the NRB case. Previous numerical studies by Balarac [7] showed that recirculation bubble contribute to the increased mixing between the annular and the central jets. Similar observations are made in the current SPRF studies. Figure 64 (a) compares the mixture fraction along the centerline in the RB and NRB cases. The mixture fraction \( f \) is computed using methane, oxidizer and product mass fractions at every grid point in the flow. Also marked on Fig. 64 (a) is the mixture fraction corresponding to the global equivalence ratio. The figure shows that the decay of \( f \) in the RB is slightly steeper than that in the NRB case suggesting that more mixing is occurring in the NRB case. A zoomed view of this plot is shown in Fig. 64 (b). Clearly, the mixture values are different due to the presence of recirculation bubble. The main difference between the \( RB \) and \( NRB \) cases is in the values of \( f \) attained in a region between 50 and 100 mm away from the injector. These values are much lower than the the mixture fraction values corresponding to the global equivalence ratio of 0.58 in the RB case. This situation can occur if the fuel supply into the combustor is intermittent. In order to understand this intermittency, contours of the near field instantaneous axial velocity are shown at two time instants (\( t = 8.1 \) and 8.6 ms.) in Figure 65. The near field flow features at both these instants are very different. At \( t = 8.1 \) ms., the backflow velocity in front of the injector is higher than the other. At this instant, the recirculation region acts as a blockage. For the fuel to flow into the combustor, it has to flow over the bubble into the oxidizer jet. It is observed in the results that the flow rate under these conditions is lower than the actual flow rate. This is due to the following reasons. The inflow conditions used are characterictic in nature; the velocity field is specified at the inflow, while the density is allowed to evolve based on the conditions prevailing inside the combustor. When the bubble is present in front of the injector tube, a low pressure wave passes through the inflow, which reduces the density (pressure and density are related by the equation of state). As a result the flow entering the combustor is lower than the actual mass flow rate. At some instants, the variation in the mass flow rate is as high as 10 %. At \( t = 8.6 \) ms., the recirculation bubble is weak. In this case, fuel flow into the combustor is higher than that at the other instant. This process results in an intermittent release of fuel from the injector, with an average that
is lower than the intended equivalence ratio. This process eventually lead to extinction in
the combustor. However, experimental studies on SPRF [10] demonstrate a stable flame. It
is not known from the measurements, whether such a recirculation bubble exists in the flow.
. The numerics appear to be very sensitive to the inflow conditions as reported in many
previous studies. The inflow conditions are of utmost importance in predicting the near
field flow features. Although, the studies only point out the momentum flux ratio, there
can be many other factors such as inflow turbulence, and the shape of the inlet velocity
profile that can affect the numerical predictions.

In the current work, the inflow conditions are implemented based on the mass flow mea-
surements at the annular inlet and at the fuel inlet. Accordingly, analytic velocity profiles
that match the mass flow rates are prescribed at the inflows. As mentioned before, the
shape of these profiles can affect the predictions. Also, there is the preheating effect in the
SPRF setup. Only the preheated temperature of the annular jet is known, while the inner
fuel is assumed to be at room temperature due to measurement complications. Preheating
increases the momentum ratio, even though the mass flow rates are maintained the same
in the preheated and non-preheated cases. So, incorporating these effects inaccurately can
affect the predictions. Thus, the boundary coditions specified in the simulations can be
very different from the actual experimental conditions, if all the above issues are not taken
into account. Since, the experimental data [10] suggests that the combustion is stable with
the flow rates used in the simulations, the current study further analyzes the results from
the case, where stable combustion is observed.

8.2 Results
8.2.1 Validations

Figure 66 shows the heat release in the non-premixed mode. Along with the LEMLES
results, the flame predictions from EBULES and steady flamelets (SFLES) from an earlier
study [117] are also shown here. Both EBULES and SFLES show a very different flame
location from the experiments. Note that, the heat release can not be computed in SFLES
due to the nature of the model. Hence mean temperature contours are shown here to
represent the flame. The high temperature regions near the injector indicate that in SFLES, combustion occurs immediately after the fuel and air mix. In the SFLES implementation, the exhaust gas dilution effects were not included in the construction of flamelet libraries. An unsteady flamelet model [64] in which non-equilibrium kinetics are taken into account may be able to handle this effect but is expensive and not explored here. The LEMLES approach (without any changes to the earlier version) captures the lifted non-premixed flame, and shows that all the heat release occurs only in the downstream region of the combustor. The rest of this study uses LEMLES results to explain the observed flame structure in the non-premixed mode.

Figure 67 compares the predicted and measured mean centerline axial velocity decay in the premixed and non-premixed cases. The non-premixed case exhibits a lower peak than the premixed case due to the presence of the low velocity inner fuel jet, which has an injection velocity of 40 m/s. This velocity in the non-premixed case decreases rapidly to a value as low as 8 m/s within the first 5 mm from the injector, and then increases to a peak value of 92 m/s at x = 60 mm. The peak velocity along the centerline is attained due to the merging of the outer jet. Figure 67 also shows that the outer jet in the premixed case merges earlier than that in the non-premixed case. The predictions in the premixed case are a little higher than the measurements while the non-premixed case predicts lower values. Beyond x = 250 mm, computations show very low velocities when compared to the measurements. This could be due to the long computation times needed to settle the flow in these regions.

Figure 68 shows the radial profiles of the mean axial velocity at different axial locations for both modes. The axial locations chosen are x = 57, 113, 187 and 245 mm. There is a good agreement between the experiments and the computations in the non-premixed case. Some discrepancies are observed between the predictions and the measurements away from the centerline at x = 57 mm. The agreement gets better as the velocity decays downstream. The velocity decay is influenced both by confinement [60] and the stagnation end plate. Some asymmetry is observed in the measurements due to the slight misalignment of the inner tube within the annular injector. Downstream of the injector, predicted and measured
velocity profiles of both modes overlap at $x = 187$ and 245 mm suggesting the qualitative similarity of the velocity field. In addition, the computed velocity profiles are similar in the near field and away from the centerline (beyond 15 mm). The same can not be concluded from the measurements due to their asymmetric nature.

Figure 69 shows the corresponding RMS axial velocity profiles. LEMLES predictions compare well with the experiments except in the shear layer at $x = 57$ mm, where measured data show RMS values as high as 50 m/s. The turbulence levels in the non-premixed mode at $x = 57, 113$ mm are slightly lower than those in the premixed case, but towards the end of the combustor, the turbulence levels become similar. Thus, RMS profiles for both modes show similar intensities suggesting that the far field is controlled more by the downstream heat release (refer Fig. 66) rather than the turbulence in the near-field of the injector.

Figure 70 shows the comparison of the predicted temperature with measurements along the centerline. The trends are rightly predicted by the computations. The computed values reaches peak values at about 225 mm from the injector. Figure 71 shows the comparison of $CO_2$ mole fraction along the centerline. The computed data agree with the measurements in the near field but the discrepancies increase with increase in the axial distance. Figures 70, 71 indicate that products are present along the centerline as early as 50 mm from the injector and these products preheat the mixture.

### 8.2.2 Analysis

Figure 72 shows the instantaneous fuel destruction rates in the premixed (PRE) and non-premixed (NP) cases. The rates in the NP case are present only downstream. Hence the flame is lifted off in the NP case, whereas it is well attached to the injector in the PRE case. To find the stand off distance, the fuel reaction rate is first spatially averaged over each cross section along the axial direction and then time averaged for 3 ms. Figure 73 shows the averaged rate plotted along the axial length of the combustor. The reaction rates peak at about 170 mm from the injector. The reactions are spread over a wide region in the combustor. Most of the reaction rates observed earlier than 100 mm are present in the shear layer where the flame starts to ignite. It is observed that the nearest flame ignition
point to the injector is around 50 mm.

Figure 74 shows the scatter plots of \(CO_2\) formation rate vs. temperature. The scatter plots are shown at two cross sections located at 50 and 70 mm away from the injector. At \(x = 50\) mm, there are very few locations and instants of time at which reactions occur. Also, reactions occur only when temperatures are beyond 1200 \(K\). At \(x = 75\), there are more instants of time when the reactions occur. The high temperature regions are present along the region where the premixed fuel and air mix with the returning products. Hence, the reactions occur in the shear layer of the oxidizer and reverse flow jet. Even though regions of high temperature are present upstream of \(x = 50\) mm, the fuel and air are not mixed near the injector. Hence, no burning occurs here. This shows that fuel and air are mixed prior to combustion in the non-premixed mode.

Scalar dissipation rate plays a critical role in non-premixed combustion [82]. It can be interpreted as the rate at which the scalar fluctuations are destroyed. This rate determines the diffusion time scale in combustion applications and controls local quenching in the flow. The scalar dissipation \((\chi)\) values are computed using the following relation:

\[
\bar{\chi} = 2D \left( \frac{\partial \tilde{f}}{\partial x_j} \frac{\partial \tilde{f}}{\partial x_j} \right) \tag{89}
\]

where \(D\) is the diffusion coefficient of the mixture fraction field. Figure 75 shows the filled contours of the scalar dissipation rate along with the contour lines of the reaction rate. The dissipation values are very high near to the injector in the fuel and air mixing layer. Immediately after the fuel and air enter into the combustor, scalar dissipation is so high that the reactions can not occur here. It remains high until about 50 mm from the injector. However, even after the dissipation values decrease to low values, reactions do not appear. Further analysis of the dissipation values did not show any particular value for the local extinction in the present simulations. The role of dissipation here is mainly responsible for the absence of the flame in the fuel air mixture very near to the injector.

The flame structure in the NP case is analyzed using the Flame index (F.I.) [73]. It is defined as,

\[
F.I. = \nabla Y_F \cdot \nabla Y_O \tag{90}
\]
where $Y_F$ and $Y_O$ are the mass fractions of the fuel and oxidizer respectively. The flame is premixed when $F.I.$ is positive and diffusion when $F.I.$ is negative. Figure 76 shows two snap shots of isocontours of the reaction rates coloured with the contours of $F.I.$ The red color region is the positive $F.I.$ region, while the blue color is the negative $F.I.$ region. Almost all the reaction rates are in the red region i.e., in the premixed region. Wherever reactions occur, the gradients of the fuel and oxidizer are in the same direction. In other words, the fuel and air are not diffusing towards each other. The figure does not show any triplet flame structure, which are often involved in the stabilization of the lifted diffusion flames [85]. It is most likely that a triplet flame like structure will not occur as the SPRF flame is like a premixed one. Thus, computations are able to predict the stabilization in the non-premixed mode in SPRF.

Based on the computed F.I. values, it is concluded that the non-premixed flame in SPRF is behaving similar to a lifted premixed flame. It would be interesting to find if the reactions occur under lean or rich conditions. To find this out, a scatter plot of the mixture fraction and the fuel destruction rate is plotted and is shown in Fig. 77. The mixture fraction values corresponding to stoichiometric and global equivalence ratios are marked in the figure. Most of the times, reactions occur under lean conditions, and sometimes near the global equivalence ratio. This again confirms that mixing of the fuel and air first occurs in the combustor and reactions occur under lean conditions in the non-premixed mode. This is in agreement with the conclusions from the experimental data [34].

Figure 78 shows the % of heat release occurring at different mixture fractions. A 14.7 % of heat release, which is the maximum value, occurs at the mixture fraction value of 0.034. This corresponds to an equivalence ratio of 0.6. Most of the heat release occurs on the lean side between the mixture fraction values of 0.03 and 0.04. These seem to be some amount of heat release occurring below the overall equivalence ratio and also on the rich side. These could be due to heat release in isolated regions of rich and lean fuel pockets in the combustor.

Mass entrainment is evaluated by computing the mass flux at different axial locations using an entrainment rate: $e = \dot{m}_e/\dot{m}_o$. Here, $\dot{m}_o$ is the inlet mass flow rate and $\dot{m}_e =$
$j_0^R 2ρ\bar{u}_rdr$, where R is defined as the location along the radial direction, where the axial velocity is zero. Figure 79 compares $e$ for both premixed and non-premixed cases. In both modes, entrainment increases initially due to the increase in mass inside the jet and the confinement [60], but decreases downstream due to velocity decay and the presence of the stagnation plate. Also, the conversion of high density reactants to low density products decreases the mass inside the forward jet. The decay of entrainment rate in the premixed mode is steeper than in the non-premixed mode due to the difference in the flame structure. In the premixed mode, combustion occurs upstream along the shear layer, whereas in the non-premixed mode, combustion occurs downstream. As a result, mass flux inside the jet decreases at a faster rate in the premixed mode.

The amount of products along the centerline are compared in Fig. 80. Upstream of $x = 75 \, mm$, there is not much difference, but further downstream, products in the premixed mode reaches saturation levels faster (around $x = 175 \, mm$, which is an indication of the mean flame length). However, in the non-premixed mode, the product concentrations continue to increase till around $x = 225 \, mm$ before leveling off. This further confirms that the flame in the non-premixed case is located further downstream (as seen in Fig. 66).

The radial profiles of $O_2$ at three axial locations are shown in Fig. 81. Peak values for the premixed case are due to the merging of the annular jet as early as $x = 30 \, mm$ from the injector. However, in the non-premixed case, the annular jet merges only later and the profile of $O_2$ in Fig. 81 is due to the rapid mixing of the annular air jet with the central fuel jet. From $x = 30 \, mm$ to $x = 120 \, mm$, oxygen in the non-premixed case spreads in the radial direction, which is not observed in the premixed case. This is related to the flame location since in the premixed case, it is along the shear layer (no reactant $O_2$ is present), while in the the non-premixed case, it is further downstream (beyond $x = 120 \, mm$) and hence oxygen shows a radial spreading in the near field.

The reactant dilution effect in the non-premixed mode is explored by looking at the instantaneous semi-logarithmic scatter plot of the fuel break-up reaction (1st step) rate against the ratio of the fuel ($CH_4$) and $CO_2$. The scatter plot is shown in Fig. 82(a). Also marked in the figure is the location at which the mixture has 50 % of reactants and 50 % of
products according to the global reaction $CH_4 + 2O_2 \leftrightarrow CO_2 + 2H_2O$. Most of the times, regions where the reactions occur correspond to regions where more than 50 % products are present. The products present at each location can be either due to the entrainment of products or due to the reactions that occurred in the previous instants.

This can be further visualized in an instantaneous iso-contour of the fuel destruction rate colored with the ratio of the fuel mass to $CO_2$ mass in Fig. 82(b). Black regions indicate less than 50 % products while white regions indicate more. Since products are present even at 5 Dia from the injector along the centerlin, the reactions occur with some product dilution as shown in Fig. 82.
Figure 63: Contours of the mean axial velocity very near to the injector. Units in m/s
(a) Centerline variation of mixture fraction in RB and NRB cases

(b) Centerline variation of the mixture fraction in the RB and NRB cases in the region where there is recirculation bubble

Figure 64: Centerline variation of mixture fraction.
Figure 65: Instantaneous contours of the axial velocity. Units in m/s.
Figure 66: Flame location in experiments [34] and different LES sub-grid closures. Heat release is used to represent the flame location except in SFLES where temperature contours are used. The units of computed heat release is $J/s$.

Figure 67: Comparison of the centerline mean axial velocity.
Figure 68: Comparison of the radial profiles of the mean axial velocity.

Figure 69: Comparison of the radial profiles of the RMS axial velocity.
Figure 70: Comparison of temperature along the centerline.

Figure 71: Comparison of carbondioxide mole fraction along the centerline.
Figure 72: Instantaneous reaction rates in the premixed and non-premixed modes. Units in $Kmol/m^3s$
Figure 73: Variation of the reaction rates along the centerline. The rates are averaged over the entire cross section at every axial location. Units of the rate is $Kmol/s$

Figure 74: Scatter plots of reaction rate vs. temperature. Units of reaction rate is $Kmol/m^3s$ and temperature is $K$
Figure 75: Filled contours of the scalar dissipation rate with contour line of the fuel destruction rate. The units of scalar dissipation is $1/s$.

(a) $t = 8.2$ ms.  
(b) $t = 12.9$ ms.

Figure 76: Isocontour of the instantaneous reaction rate colored with F.I.. Color red denotes +ve F.I. and color blue denotes -ve F.I.
**Figure 77:** Scatter plot of fuel destruction rate vs mixture fraction. Units of fuel destruction rate is $Kmol/m^3s$.

**Figure 78:** Variation of the % of the heat release with the mixture fraction.
Figure 79: Entrainment rates for the reacting cases.
**Figure 80:** Centerline variation of the products mole fraction.

**Figure 81:** Radial profiles of $O_2$. 
(a) Scatter plot of Fuel destruction rate vs $CH_4/H_2O$ ratio. The $y$ axis is in logarithmic scale. Units of the rate is $Kmol/m^3s$.

(b) Isocontour of the fuel destruction rate colored with values of $CH_4/CO_2$.

Figure 82: Dilution in the non-premixed mode.
CHAPTER IX

CONCLUSIONS AND FUTURE WORK

9.1 Conclusions

The primary goal of this work is to understand flow features and combustion phenomenon in Stagnation Point Reverse Flow (SPRF) combustor. In the SPRF combustor, the inflow and the outflow are on the same side of the combustor. Therefore, the mixing between the hot products and the incoming reactants occurs as an internal mechanism. The flame stabilization mechanism in SPRF, at very lean conditions, produces very low emissions in both the premixed and non-premixed modes. Experimental investigations showed that the flame structure is similar in both the modes, with some differences near the injector. The current work aims to resolve all these features in the SPRF configuration using Large Eddy Simulations (LES) as the numerical tool.

From combustion modeling point of view, different closure models are available in the literature to mimic the interaction between turbulence and chemistry. The choice of the closure should depend on the information that is required from the simulation. Also, the available computational resources will effect the choice. In the premixed combustion mode, simple chemistry closures such as Eddy Break-Up Model (EBULES) and artificial Thickened Flame (TFLES) predicted the velocity field reasonably well in most parts of the combustor. However, the prediction of the combustion characteristics such as heat release and flame structure are not accurate. These predictions depend entirely on the inherent assumptions used while deriving the closures, and should be validated for different combustion regimes. It is, however, possible to make ad hoc changes to these models to obtain better predictions. It is shown in the current work that, for the accurate predictions using TFLES approach, the reaction rates in the regions of high temperature and low amount of the reactants must be accurately computed. It is also shown here, particularly for the SPRF combustor, that the sub-grid scale combustion model employed for LES should be able to resolve the sub-grid
molecular diffusion, chemical reaction and turbulent stirring in an effective way to provide accurate results. An approach known as LEMLES, which accounts for these effects, was shown to accurately predict both the flow and the scalar fields without any modification to the previous model formulation. The same implementation of LEMLES was observed to capture the combustion phenomenon accurately both in the premixed and non-premixed modes. This establishes that the LEMLES approach can be used in this novel configuration without requiring additional changes.

The SPRF design incorporates confinement, flow reversal, same side inflow and outflow design and a stagnation end plate. Thus, the flow features observed here are a combination of all the above features. It has been proven that the mass entrainment is present in all the cases studied and the amount of mass entrained is shown to be proportional to the radial velocity induced in the flow. The radial velocity is found to be the highest very near the injector, which suggests that the entrainment of mass is highest close to the injector. The entrainment is found to be absent beyond the vortex core, more specifically beyond the intersection point of the zero axial velocity and the zero radial velocity. Beyond the vortex core, the radial velocity is pointed away from the jet center and hence there is no entrainment. Similar trends are present in the reacting cases. Even though the radial velocities are higher in the reacting case, the entrainment levels are lower than that calculated for the non-reacting case. This is a result of the lower density of the entrained mass in the reacting cases. Also, the mass entrainment in the SPRF setup reaches higher values much earlier (closer to the injector) than that in a momentum driven jet.

The entrained mass in the reacting flows carried hot products into the reactant stream. As a result, products are observed along the centerline as early as 5 diameters (air tube) away from the injector. In the premixed reacting case, the flame can potentially block the products from entering into the reactant stream. A number of broken zones are observed on the flame surface and through these broken zones, the products are able to enter into the flame. This is the mechanism through which the product gas recirculation occurs in the SPRF premixed flame. The hot products increase the temperature of the reactants. The high preheat temperature, in turns, increase the reactivity of the mixture, which resulted in
an efficient burning of the lean mixture. Analysis of the flame structure showed that most of the combustion process occurs in the thin reaction zone regime with two exceptions. The part of the combustor close to the injector exhibits isolated broken reaction zones, where as farther downstream of the combustor, combustion occurs closer to the laminar flamelets regime. It has been shown that, the turbulent eddies close to the injector are very small and can penetrate into the reaction zone. Further downstream, the reactivity of the mixture increases and the turbulent structures get larger. Hence, the flame speeds are higher and the turbulence effects are minimal on the flame.

The application of a complex chemical kinetics mechanism is also discussed in this work and the results are compared with those obtained by using a two step reduced global mechanism. The velocity predictions differed little with the detailed chemistry when compared with the simple kinetics. However, the turbulence predictions in the near field are better in this case. The detailed chemistry case predicted more number of local extinction zones in the near field and hence predicted low heat release, which is in agreement with the experiments. Other than that, the results are not very different from the reduced chemical mechanism studies. The flame structure was initially thought to be the reason for the underprediction of product entrainment as the products are found to enter into the flame through the broken zones. However, the detailed chemistry also predicted similar entrainment levels in the near field. This suggests that even though there are more broken zones on the surface, the product entrainment is not high. The same entrainment in both simple and complex cases is attributed to the same level of radial velocity predictions in both the cases.

Global one step models for thermal and non-thermal $NO_x$ are able to predict the emissions in the premixed reacting cases. The primary reason for low $NO_x$ is due to the ability of the combustor to burn under very lean conditions. The lean mixtures produced low temperatures and hence low thermal $NO_x$. The computed results conclude that the $NO_x$ emissions by both non-thermal and thermal pathways are of same magnitude. Since the simulations use adiabatic wall boundary conditions, it is likely that the thermal $NO_x$ predictions in the computations are high, which leads to the conclusion that the non-thermal $NO_x$ dominates.
the \( NO_x \) formation under the SPRF operating conditions. It is also observed in the SPRF setup that the residense times needed to obtain a statistically stationary \( NO_x \) is longer than that required for the flow. Also shown in this work is that a simple emission model for \( CO \) could not predict appropriate \( CO \) emissions. Only a detailed chemical mechanism for \( CO \) produced appropriate levels.

In the non-premixed mode, the inflow boundary conditions played a very important role in the evolution of the flow near the fuel injector. In particular, the momentum flux ratio between the air jet and the fuel jet was found to influence the near field flow. A recirculation bubble is shown to form in front of the fuel inlet in a low momentum case. This impacted the mixing pattern in the near field. In this case, the bubble is observed to cause flow rate oscillations at the fuel inflow. Hence, in the non-premixed case, the near field predictions are observed to be very sensitive to the inflow conditions.

The non-premixed flame is a lifted one with most of the heat release occurring in the second half of the combustor. The lifted non-premixed flame is observed to exhibit similar characteristics with a premixed flame, i.e., the flame stabilization mechanism is like a premixed flame without any triplet flame like structure which is relevant for the non-premixed flames. The flame is stabilized in beyond 70 \( mm \) from the injector in the regions where the temperatures are high and that the fuel and air are mixed. This is demonstrated using the mixture fraction, which is shown to drastically decrease in the first 70 \( mm \) and reach lean conditions. It is under these lean conditions that burning occurs in the non-premixed mode. Most of the heat release also occurs on the lean side with maximum value at \( \phi = 0.06 \). Computations show that reactions do not occur without the premixing of the fuel and oxidizer. In addition, the entrainment of products leads to mixing of the reactants with the products. The products increase the temperature of the products and provide the necessary stabilizing effects. Thus, a stable combustion phenomenon is observed even after premixing to very lean conditions in the SPRF configuration.
9.2 Future work

The LEMLES studies presented in the thesis for different combustion modes demonstrated the capability of the model to capture the correct physics to some extend. However it should be noted that, although the sub-grid scale combustion model used in the thesis is proved to be working fairly well, there is still some room for modifications related with the other aspects of the computation, and for some further study to analyze the flow features within the combustor under different conditions. These proposed studies are outlined briefly below.

**TFLES studies** The current studies with TFLES approach has shown that the reaction rate computations are not right in the regions where there are high temperatures with some reactants. In such regions, the computed flame thickening factors are high leading to very large chemical times. A recommendation is to restrict the flame thickening factors in such regions. Future studies should include these changes.

**Heat losses** The local extinction zones near the injector are shown to entrain the products. Heat losses at the injector play an important role in the accurate predictions of these local extinctions. Hence, the numerical simulations should include a heat loss model at the injector tip.

**Heat transfer** The reactant jet is preheated by the flow of products over the injector. These preheating conditions are explicitly included in the simulations by modifying the inflow conditions. However, current experimental studies showed that the flow evolution in the near field is very sensitive to the inflow conditions. Hence, incorporating the heat transfer across the injector walls can lead to more realistic exit conditions at the injector.

**TFLES studies in Non-premixed mode** The current studies showed that the flame structure in the non-premixed mode is like a premixed flame. Hence, the TFLES approach, which is developed for the premixed mode can be used to study the non-premixed flame in the SPRF combustor. This study is recommended in future.

**Parametric studies** The velocity field and the combustion field in the current studies are studied for one particular configuration of the SPRF setup. However, the effects of changing the combustor length and the outer tube diameter on these processes must be investigated.
using numerical approaches. The confinement and the stagnation end plate can change the product entrainment and hence affect the flame stability and emissions. Also, computations must also be performed at different equivalence ratios to understand the effects of heat release on the velocity field. In addition, the flow and thermal field must be investigated at different flow rates.

**Computation of reaction rates** More than 50% of the time is spent on computing the reaction rates in the LEMLES approach. This holds a limitation on the chemical kinetics employed in the studies. Methods like Artificial Neural Networks (ANN) must be incorporated in these studies to speed up the computation times, which would lead to use relatively higher order chemical kinetics mechanisms without increasing the computational burden further.

**Pollutants** Appropriate emission mechanisms must be included to predict the emissions in the current studies.

**High pressure studies** Practical combustors operate at high pressures. The current work demonstrates that LEMLES is able to predict the combustion phenomenon at atmospheric conditions. There is definitely a need to test this setup at high pressure for it to become operational. Hence LEMLES studies at high pressures should be performed.

**Liquid fuel injection** Although gaseous fuels are suitable in many applications, liquid fuel combustion is preferred in aircraft turbine engines. Hence, a computation study with liquid fuel is also recommended for future studies.
REFERENCES


165


