ABSTRACT

KUNDU, PRITHWISH. Tabulated Combustion Model Development For Non-Premixed Flames. (Under the direction of Dr. Alexei Saveliev and Dr. Tarek Echekki.)

Turbulent non-premixed flames play a very important role in the field of engineering ranging from power generation to propulsion. The coupling of fluid mechanics and complicated combustion chemistry of fuels pose a challenge for the numerical modeling of these type of problems. Combustion modeling in Computational Fluid Dynamics (CFD) is one of the most important tools used for predictive modeling of complex systems and to understand the basic fundamentals of combustion. Traditional combustion models solve a transport equation of each species with a source term. In order to resolve the complex chemistry accurately it is important to include a large number of species. However, the computational cost is generally proportional to the cube of number of species. The presence of a large number of species in a flame makes the use of CFD computationally expensive and beyond reach for some applications or inaccurate when solved with simplified chemistry. For highly turbulent flows, it also becomes important to incorporate the effects of turbulence chemistry interaction (TCI). The aim of this work is to develop high fidelity combustion models based on the flamelet concept and to significantly advance the existing capabilities. A thorough investigation of existing models (Finite-rate chemistry and Representative Interactive Flamelet (RIF)) and comparative study of combustion models was done initially on a constant volume combustion chamber with diesel fuel injection. The CFD modeling was validated with experimental results and was also successfully applied to a single cylinder diesel engine. The effect of number of flamelets on the RIF model and flamelet initialization strategies were studied. The RIF model with multiple flamelets is computationally expensive and a model was proposed on the frame-
work of RIF. The new model was based on tabulated chemistry and incorporated TCI
effects. A multidimensional tabulated chemistry database generation code was developed
based on the 1D diffusion flame solver. The proposed model did not use progress variables
like the traditional chemistry tabulation methods. The resulting model demonstrated an
order of magnitude computational speed up over the RIF model. The results were val-
ified across a wide range of operating conditions for diesel injections and the results
were in close agreement to those of the experimental data. History of scalar dissipation
rates plays a very important role in non premixed flames. However, tabulated methods
have not been able to incorporate this physics in their models. A comparative approach is
developed that can quantify these effects and find correlations with flow variables. A new
model is proposed to include these effects in tabulated combustion models. The model
is initially validated for 1D counterflow diffusion flame problems at engine conditions.
The model is further implemented and validated in a 3D RANS code across a range of
operating conditions for spray flames.
DEDICATION

This work is dedicated to my parents.
BIOGRAPHY

The author started graduate school in the Masters program in Mechanical Engineering in 2010 at North Carolina State University under the guidance of Dr. William Roberts and worked on gas turbine combustion. He graduated with a MS in Mechanical Engineering in 2012 and then started his PhD program in Aerospace Engineering in the same university. The PhD work continued with turbulent combustion modeling under the guidance of Dr. Tarek Echekki and Dr. Alexei Saveliev. The final dissertation work presented is a result of the academic and lab work done in the field of combustion over these 5 years.
ACKNOWLEDGEMENTS

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“For the strength of the Pack is the Wolf, and the strength of the Wolf is the Pack.”
- Rudyard Kipling.
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Chapter 1

INTRODUCTION

1.1 Engine Combustion Modeling

Combustion is one of the most interesting and important phenomena occurring in natural and man-made processes. In the past few decades, researchers around the world have invested significant resources to understand the complex processes associated with combustion. Many combustion applications that are of importance occur in the turbulent flow regime, which further increases the intricacies of the problem. Computational Fluid Dynamics (CFD) provides a better understanding of this complicated phenomenon of turbulent combustion for applications where experimental methods are not able to visualize flow-fields easily. It also provides an opportunity to test and validate theories and/or models against available experimental data, thus pushing towards predictive simulation capabilities. A similar approach has been used in the engine modeling community. One example that has drawn lots of attention recently is the Engine Combustion Network (ECN) [1].
1.2 Combustion Modeling of Spray Flames

A number of flamelet-type models have been used to model Spray H and Spray A recently. Ayyapureddi et al. [2] used the Flamelet Generated Manifold (FGM) combustion model coupled with Reynolds-Averaged Navier-Stokes (RANS) approach to simulate Spray A. FGM assumes the chemistry parameterized with the mixture fraction and a flamelet progress variable coupled with a beta function. Lift-off lengths were predicted for different ambient temperature and density conditions, and reasonable agreement was obtained compared to the measurement. The model was further extended within a Large-Eddy Simulation (LES) framework by Bekdemir et al. [3] to simulate Spray H; good predictions for the spray and flame characteristics were observed. Azimov et al. [4] studied Spray H with the three zone extended coherent flamelet model (ECFM3Z) developed by Colin and Benkenida et al. [5]. The ECFM3Z model divides each computational cell into 3 sub-grid regions in the mixture fraction space as unmixed fuel region, mixing region with fuel, and air and residual gases. The effect of change in lift-off lengths, pressure traces and heat release rates were compared with measurements for different ambient oxygen and density conditions. The results showed that this model was able to predict better lift-off lengths for higher oxygen concentrations and under-predicts the lift-off lengths at lower oxygen concentrations. The most relevant work for the present study is that by DErrico et al. [6], who implemented a multi-flamelet representative interactive flamelet (RIF) model coupled with RANS in OpenFOAM solver and compared the results to a well-mixed model for variations of ambient temperature and oxygen conditions. Qualitatively and quantitatively better estimations were obtained with the RIF model compared to the well-mixed model. Bolla et al. [7] studied Spray H with the Conditional Moment Closure (CMC) model coupled with RANS on a 2D grid. Lift-off length and
soot formation were studied at different ambient densities and temperatures. Bottone et al. [8] then applied this CMC model to simulate Spray H in a LES modeling framework. The ignition delays and lift-off lengths were found to be in good agreement with the experiments. Bhattacharjee and Haworth [9] and Pei et al. [10–12] used the transported probability density function (TPDF) model coupled with RANS turbulence model to simulate Spray H and Spray A on a 2D grid. Their results showed significant differences between predictions by the well-mixed and TPDF models. The flame structures predicted by the well-mixed models were unrealistically thin compared with those predicted by the TPDF model. Moreover, quantitatively more accurate results were observed with the TPDF model. Some of these studies have demonstrated the efficacy of the TCI modeling approaches by comparing them to a well-mixed type of approach. However, comprehensive studies that systematically evaluate the effect of TCI for spray flames accounting for numerical artifacts (such as grid convergence, dimensionality effects i.e., 2D vs. 3D) and chemical kinetic mechanism effects are very few in number. This motivates our current study with the multi-flamelet RIF model. The objective is to evaluate a high-fidelity RIF model over a wide variety of ambient conditions for Spray A, which includes different ambient temperatures, oxygen concentrations, densities, and injection pressures. The effect of the number of flamelets in the RIF model was investigated to understand the minimum number of flamelets required to correctly resolve the flow. The role of the presumed forms of scalar PDFs was also studied in detail. Results were also examined by bypassing the PDF integration process in order to neglect the effect of the mixture fraction variance. Simulations were also carried out to investigate the effect of different reaction mechanisms. The main focus of this part is to establish the best practices for using RIF in spray flames and to improve the efficacy of RIF calculations.
1.2.1 Challenges in Combustion Modeling

One of the major challenges in high fidelity combustion modeling is the computational cost. Large chemistry mechanisms are required to model the transient effects and pollutant formation. However, with finite-rate chemistry models a transport equation needs to be solved for each specie. This increases the computational cost for combustion applications with complex chemistry. This complexity coupled with the other complexities of turbulent spray modeling make high-fidelity simulations difficult. Flamelet models have been able to address this problem efficiently and solve a number of complex problems with relatively large chemical mechanisms. The flamelet model computes chemistry in a 1D space based on mixture fraction decoupling the fluid flow from the chemistry. This removes the stiffness of the system. Flamelet libraries can be generated before runtime and then used in the reacting flow simulations as look-up tables. The various implementations of this modeling approach coupled with the assumptions has given rise to a number of tabulated flamelet models. The steady laminar flamelet model assumes steady behaviour of the flamelet and is one of the early implementations of tabulated flamelet models. However, a steady flamelet library cannot model unsteady chemical kinetics. Thus, a number of tabulated flamelet models based on progress variables have been developed to describe the chemistry transition from unburnt state to burnt state. The progress variable describes the progress of combustion from unburnt to burnt state based on the evolution of a few species. Moreover, transport equations need to be solved for these variables. There exists a need to develop modeling techniques with tabulated flamelet models without the use of progress variables, and this has been one of the major tasks of this study.
1.2.2 Unsteady Strain Effects

It has been shown in many experimental and numerical studies that non-premixed flames are subject to unsteady strain effects. These unsteady effects can affect species production, auto-ignition and extinction. These effects cannot be captured using tabulated models. Tabulated models calculate species mass fractions based on the independent variables of the current time step. These unsteady effects have significant influence on ignition and extinction and need to be systematically evaluated. Moreover, the variables affecting these effects need to be quantified. The dissertation tries to quantify these effects and develops modeling approaches that can consider these effects in tabulated models.

The influence of fluctuating strain on flames with respect to ignition, extinction and species concentration has been the focus of numerical and experimental work by many researchers in the past decades. Peters and William [13] discussed a flame stabilization mechanism for non-premixed counter flow diffusion flames (CFDF) based on quenching limits of flamelets and their dependence on scalar dissipation rate (SDR). This was also supported by findings of Mastorakos et al. [14]. Egolfopoulos et al. [15] numerically studied 1D CFDF with sinusoidal velocities. The flame response was quasi steady for very high and very low frequencies. However, the intermediate frequencies showed a phase shift between the oscillations and the flame response. Similarly Kistler et al. [16] carried out experimental and numerical study of CFDFs and observed that for very low and high frequencies in strain oscillations the behaviour was quasi steady. Extinction was not observed for very high frequencies with peak strain values beyond quenching limits. Im et al. [17] studied CFDFs under oscillating strain with similar conclusions. It was suggested that as the strain rate increases beyond the extinction limits the flamelet needs some time to respond to this rapid change. If the time scale of oscillation is not long enough
then these high strain rates are not sufficient for the flame to extinguish. Similar results were observed by Brown et al. [18]. Barlow et al. [19] studied the effect of a temporal step change (sudden decrease) of strain on flamelets experimentally as well as numerically using the steady flamelet assumption. The results showed that the steady flamelet assumption over predicted the OH and CO species concentrations. This showed the significance of the history effects on a flamelet. These studies suggested the importance of unsteady effects in flamelets and the inadequacies of the steady strain assumption to predict flame response under temporally changing SDRs. In this study these unsteady effects will be referred to as the history effects.

Tabulated flamelet models have been used extensively and have successfully reduced computational costs. The progress-variable type unsteady models, which can take into account unsteady chemical kinetics, cannot account for the effect of strain rate history. Researchers in the past few years have tried to address this problem. Cuenot et al [20] proposed the idea of calculating an equivalent strain based on the history of a flamelet. For a CFDF with oscillating strain this equivalent strain was used in conjunction with steady flamelet libraries. The equivalent strain accounted for the history effects of the flamelet. Results showed that this concept can be used to predict accurate results for a flamelet with oscillating strain using steady flamelet libraries. This formulation and its validation was based on single-step chemistry and a single time scale. For chemistry involving multiple species an equivalent strain needs to be calculated for each specie. Moreover, if there are multiple reactions with production and consumption for each specie then correction factors need to be calculated for the production and consumption rates. This would add significant complexity for detailed hydrocarbon mechanisms with hundreds of species and reactions. Delhaye et al. [21] developed a framework to incorporate unsteady effects in flamelet generated manifolds. A 2 dimensional FGM manifold was was
used to predict species for a CFDF with oscillating strain and compared with detailed unsteady simulations using GRI 3.0 chemistry for methane. The 2D manifold predictions showed a phase shift with the detailed simulation. A 3D manifold was then created where the chemistry was a function of 3 controlling variables. This manifold was generated by running a number of CFDF problems with varying amplitude and frequencies of strain oscillations. No phase shift was observed between predictions from the 3D FGM manifold and the unsteady results. The work was further extended to extinction limits in [22].

The numerical and experimental studies so far dealt with oscillating strain on flamelets in the context of turbulent gas jet flames with CH$_4$ chemistry at 1 atm pressure. The temporal variations in SDR studied are of sinusoidal nature. However, the temporal variations observed in spray flames have a different behaviour. This was reported in [23] and also by D’Errico et al. [24]. The scalar dissipation rates in spray flames for flamelets experience much larger gradients and decay exponentially over a short period of time as the flamelet like structures move away from the nozzle. The main aim of the study is to study the unsteady effects in flamelets and their influence on auto-ignition and flame stabilization under such high pressure engine conditions for diesel surrogates with detailed chemistry mechanisms. A systematic approach needs to be developed that can quantify these history effects in flamelets and identify variables that influence these effects. This understanding can help develop modeling approaches that incorporate history effects in tabulated models. Moreover, such models have not been applied and validated for real 3D CFD spray flame simulations. The goal is to implement and validate modeling concepts that can incorporate history effects in tabulated combustion models.
1.2.3 Engine Combustion Network Spray A

Consistent and reliable experimental data are a prerequisite for validating simulation models. These experiments span a wide range of fuels and configurations. It is necessary to have a very good understanding of the boundary and operating conditions. Internal combustion engines usually operate at elevated temperatures and pressures. The construction of the combustion chamber is usually very complex and inaccessible to optical sensors and instruments. Moreover, the length and time scales of turbulent fluid dynamics and combustion necessitate spatial and temporal data with very high resolutions. All these factors make it extremely difficult to obtain accurate experimental data for turbulent flames at higher pressures. A number of experimental methods have been developed by the scientific community and have been applied to turbulent non-premixed flames. Also there are a wide range of models to account for different physics like spray physics, turbulence, combustion models and chemistry. These have been implemented across a wide range of codes and modeling techniques. It is beneficial to have a common understanding of these experiments and modeling approaches. Standardized experimental conditions would allow comparative study between different modeling frameworks and codes and establish best practices. This approach has been used in the engine modeling community. One example that has drawn lots of attention recently is the Engine Combustion Network (ECN) [1]. This chapter also provides an overview of the experiments with non-premixed diesel spray combustion at conditions that mimic diesel engine conditions. Emerging trends in advanced engines involve fuel injection at relatively lower temperature conditions. The ignition delays are longer for these conditions and auto-ignition is dominated by the low-temperature reactions. Thus, the unsteady chemical kinetic effects and reaction mechanisms play important roles in modeling the auto-ignition phenomenon.
This coupled with the physics of turbulent mixing makes it difficult to model and understand the auto-ignition and flame stabilization phenomena. Spray A focuses on conditions that involve exhaust gas re-circulation in the low temperature combustion regime. A wide range of parametric variations have been carried that cover a wide range of diesel engine conditions. The modeling setup of Spray A is then discussed in the context of a 3D RANS code. This model set up is then validated against experimental data across a wide range of conditions. Further model development, implementation and validations are based on this Spray A setup.

The ECN provides a platform to enhance the collaboration between experimentalists and modelers to further understand the complicated combustion behaviour under diesel engine conditions. This involves injecting a fuel spray into a high temperature, high-pressure constant-volume combustion chamber that mimics the conditions of a diesel engine. N-heptane and n-dodecane have been used as diesel fuel surrogates and studies under a specific set of conditions using a single-hole injector have been named Spray H and Spray A, respectively. Various measurements have been obtained from these experiments over a wide range of conditions with different experimental techniques [25–28]. Many research groups worldwide have also been modeling these spray flames with different combustion models in various codes using different reaction mechanisms. Some of them used the traditional well-mixed combustion model with finite-rate chemistry [29–32], which neglects the effect of turbulence-chemistry interaction (TCI) and uses the cell-averaged temperature, pressure, and species concentration for the chemical source term calculations. However, neglecting the turbulence fluctuations (e.g., temperature) could result in errors under some conditions due to the high non-linearity of the chemical source term, which is exponentially dependent on the temperature. There is a need for combustion models that account for the effect of TCI for improving the accuracy of
1.2.4 Spray A Experimental Setup

The experimental setup consists of a constant-volume combustion chamber, with either ignition of a premixed fuel-air mixture [25] or preheated compressed air [27] used to achieve the target ambient conditions. Once the desired conditions are reached, the fuel is injected into the constant-volume chamber through a single-hole injector. Some important parameters from the experiments are summarized in Table 1.1. The constant volume combustion chamber is equipped with optical access, which enables a wide range of diagnostic measurements. Liquid penetration length, ignition delay and flame lift-off lengths are measured for different operating conditions. Ignition delay was measured by looking at the pressure rise data and OH chemiluminescence was used to find the lift-off lengths.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quantity</th>
<th>Baseline case conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>n-dodecane</td>
<td>n-dodecane</td>
</tr>
<tr>
<td>Nozzle outlet diameter</td>
<td>90 microns</td>
<td>90 microns</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.86</td>
<td>0.86</td>
</tr>
<tr>
<td>Fuel Injection Pressure</td>
<td>50-150 MPa</td>
<td>150 MPa</td>
</tr>
<tr>
<td>Injection Duration</td>
<td>1.5 ms</td>
<td>1.5 ms</td>
</tr>
<tr>
<td>Injected fuel mass</td>
<td>3.5 mg</td>
<td>3.5 mg</td>
</tr>
<tr>
<td>Ambient gas temperature</td>
<td>800-1200K</td>
<td>900K</td>
</tr>
<tr>
<td>Ambient gas density</td>
<td>15.7-22.8 kg/m³</td>
<td>22.8 kg/m³</td>
</tr>
<tr>
<td>Ambient oxygen concentration</td>
<td>13-21</td>
<td>15</td>
</tr>
</tbody>
</table>
1.3 Dissertation Objectives

The challenges to turbulent combustion modeling are evaluated in this work. The main objective is to develop models that can address these challenges at lower computational costs. The objectives are summarized as follows:

- Evaluate RIF model for turbulent spray flames over a wide range of conditions. Investigate the effect of turbulence-chemistry interactions for high pressure, turbulent spray flames. Determine the effect of number of flamelets and evaluate strategies to determine optimum number of flamelets. Then, evaluate these modeling strategies for a single cylinder diesel engine case.

- High fidelity combustion models with large chemistry mechanisms are computationally expensive. The goal is to develop a novel tabulated combustion model capable of incorporating unsteady chemical kinetics with large mechanisms at lower computational costs. The main feature of the new modeling technique is to implement a model without the use of a progress variable.

- Tabulated models have relatively lower computational cost, however, they cannot account for unsteady effects. These unsteady effects have not been evaluated for high pressure spray flame configurations. The quantification of these unsteady terms is important to develop tabulated models that can account for unsteady strain effects. Development of such modeling techniques will lead to high fidelity combustion models that are computationally cheaper and account for more physics than the current models.

The second chapter of the describes the modeling setup and approach for spray combustion in a RANS code available with CONVERGE. The third chapter describes
the implementation of the Representative Interactive Flamelet model available with the CONVERGE code. The RIF model is validated across a wide range of Spray A conditions and a single cylinder diesel engine. An approach to determine the number of flamelets is developed. The conclusions from the constant volume combustion vessel are found to be consistent with the findings from the single cylinder diesel engine simulations. These results show the implementation of a high fidelity flamelet model capable of solving flamelet histories with the use of online libraries.

The development of the tabulated model based on the RIF framework and its implementation with the 3D CFD code is discussed in the fourth chapter. The chemistry tabulation process and the development of a parallel code is discussed in this section. This modeling approach is then validated across a wide range of Spray A conditions for a 106 species n-dodecane reaction mechanism. The differences between these results and the RIF model highlight the effect of unsteady strain effects on flamelets and provides further motivation to understand unsteady effects in flamelets. The fifth chapter describes the factors influencing unsteady effects in flamelets and modeling approaches for tabulated models to capture such effects. These models are then coupled with the 3D RANS code and validated across a range of conditions in Spray A. The conclusions of the dissertation are discussed in chapter 6.
Chapter 2

CFD Model Set Up for Spray Flames

2.1 Model Setup in 3D RANS Code

A commercially available CFD code CONVERGE [33] (version 2.1) was used to simulate the fuel spray and combustion processes. It uses an innovative, modified cut cell Cartesian technique to generate the grid at run time. All the simulations are performed in 3D, and the grid shown in Figure 2.3 is generated internally at run time by the code and automatically refined at certain regions based on the physics of the problem. This is achieved using adaptive mesh refinement (AMR). The gas phase is treated as a continuous Eulerian phase and the liquid spray is treated as discrete Lagrangian parcels. The source code for CONVERGE is implemented in C with Message Passing Interface (MPI) implementation for parallel processing. In-house codes for combustion models were developed in C and interfaced with the source code in a parallel environment. This type of setup enabled the implementation and validation of new combustion models for turbulent
spray combustion problems. The simulations were run on a high performance computing cluster following best practices established in [34].

### 2.1.1 Governing Equations

The following governing equations are solved in the CFD code in addition to the combustion models which will be discussed in detail. The Reynolds-Averaged Navier-Stokes (RANS) equation framework has been used in this work to model turbulent flows. Continuity and momentum equations for compressible flow are shown in Equations 2.1 and 2.2 respectively where $\rho$ is the density, $u$ is the velocity, $P$ is the pressure and $S$ is the source term in continuity equation.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = S \tag{2.1}
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + M_i \tag{2.2}
\]

The stress tensor is given by

\[
\sigma_{ij} = \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] + \left[ \mu' - \frac{2}{3} \mu \right] \left[ \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] \tag{2.3}
\]

Where $\mu$ is the viscosity and $\delta_{ij}$ is the Kronecker delta. $u$ is the velocity, $\rho$ is the density. $M$ is the source term in momentum equation.

The energy equation is given by

\[
\frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + Q \tag{2.4}
\]
where $Y$ is the mass fraction of specie $m$, $D$ is the mass diffusion coefficient.

The finite-rate chemistry combustion model is implemented by solving transport equations for each specie as shown in Equation 2.5 where $\omega_m$ is the source term for specie $m$ and $\rho_m = \rho Y_m$. This model does not consider the turbulence-chemistry interactions. The other combustion models and the ones developed are discussed in detail in the proceeding chapters.

\[
\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_m \frac{\partial Y_m}{\partial x_j} \right) + \omega_m
\]  

(2.5)

### 2.1.2 Turbulence Model

The implementation of Re-Normalization Group (RNG) k-epsilon model in CONVERGE is discussed in this section. The flow variables are decomposed into an ensemble mean and fluctuating term as shown in Equation 2.6.

\[
u_i = \bar{u}_i + u'_i
\]  

(2.6)

This decomposition when substituted into the Navier-Stokes equations give the compressible RANS mass and momentum equations as shown in Equation 2.7 and 2.8.

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = 0
\]  

(2.7)

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i u_j}{\partial x_j} = \frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right] + \frac{\partial}{\partial x_j} \left( -\bar{\rho} u'_i u'_j \right)
\]  

(2.8)

where $\bar{u}_i \equiv \frac{\rho \bar{u}_i}{\bar{\rho}}$ and the Reynolds stress is given by $\tau_{ij} = \bar{\rho} u'_i u'_j.$
The modeled Reynolds stress for the RNG model is given by 2.9.

\[
\tau_{ij} = 2\mu_t S_{ij} - \frac{2}{3}\delta_{ij} \left( \rho k + \mu_t \frac{\partial \bar{u}_i}{\partial x_i} \right)
\]  
(2.9)

where turbulent viscosity is given by \( \mu_t = c_{\mu}\rho \frac{k^2}{\varepsilon} \) and turbulent kinetic energy (TKE) as \( k = \frac{1}{2} \bar{u}_i' \bar{u}_i' \). The strain rate tensor is given by Equation 2.10

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]  
(2.10)

Turbulent diffusion and conductivity are given by Equations 2.11 and 2.12 respectively where \( Sc_t \) is the turbulent Schmidt number and \( Pr_t \) is the turbulent Prandtl number.

\[
D_t = \left( \frac{1}{Sc_t} \right) \mu_t
\]  
(2.11)

\[
K_t = \left( \frac{1}{Pr_t} \right) \mu_t c_p
\]  
(2.12)

The transport equations for turbulent kinetic energy \( (k) \) and dissipation of TKE \( (\varepsilon) \) are given by Equation 2.13 and 2.14 respectively.

\[
\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr_k} \frac{\partial k}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr_k} \frac{\partial k}{\partial x_j} \right) - \rho \varepsilon + S_s
\]  
(2.13)

\[
\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho u_i \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) - c_{\varepsilon 3} \rho \varepsilon \frac{\partial u_i}{\partial x_j} + \left( c_{\varepsilon 1} \frac{\partial u_i}{\partial x_j} \tau_{ij} - c_{\varepsilon 2} \rho \varepsilon + c_s S_s \right) \frac{\varepsilon}{k} - \rho R
\]  
(2.14)

where \( R \) is given by
\[ R = \frac{C_\mu \eta^3 (1 - \eta/\eta_0) \varepsilon^2}{(1 + \beta \eta^3)} \frac{k}{\varepsilon} \]  
(2.15)

\[ \eta = \frac{k}{\varepsilon} \mid S_{ij} \mid \]  
(2.16)

The modeling constants for the RNG turbulence model for the spray flame simulations in this study were set as \( C_\mu = 0.0845 \), \( c_{\varepsilon 1} = 1.42 \), \( c_{\varepsilon 2} = 1.68 \), \( c_{\varepsilon 3} = -1.0 \) and \( \beta = 0.012 \).

### 2.1.3 Spray Model

Injection of high pressure liquid fuel sprays in a turbulent atmosphere is modeled in the CONVERGE code. A number of factors affect spray physics and evaporation processes of the liquid fuel. This further influences the fuel air mixing process. The modeling of spray has a direct impact on auto-ignition, flame stabilization and species formation processes. The Lagrangian-Eulerian approach is used to model sprays in CONVERGE where the liquid phase is modeled as Lagrangian particles. The schematic in Figure 2.1 shows the different process that need to be modeled for any given spray combustion problem. The fuel spray coming out of the nozzle will be characterized by the radius of the droplets coming out of the nozzle. This is modeled by the primary breakup model. These liquid spray droplets further breakup into smaller droplets depending on a number of factors including aerodynamic drag, instabilities and shape of the droplet. This is modeled using a secondary breakup model. The collision between these droplets can have a significant impact on sprays. These liquid droplets are also subject to evaporation and eventual mixing with the oxidizer. All these coupled process require an accurate spray model.

The injection was modeled using the blob injection model \([35]\) where the initial droplet size of the injected fuel is equal to the nozzle hole diameter. A single component liquid
fuel ndodecane was used for this study. The liquid properties are supplied to the code in the form of a 'liquid.dat' text file. The rate of injection (ROI) was implemented for the Spray A case from available experimental data and is shown in Figure 2.2.

The Kelvin-Helmholtz (KH) [36] and the Rayleigh-Taylor models were used for droplet
Table 2.1: Under-relaxation factors and convergence criteria for different equations.

<table>
<thead>
<tr>
<th>Equation</th>
<th>Under-relaxation</th>
<th>Convergence criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1.6</td>
<td>$10^{-7}$</td>
</tr>
<tr>
<td>Momentum</td>
<td>1.0</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>Energy</td>
<td>1.0</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>Mass</td>
<td>1.0</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>Species</td>
<td>1.0</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>Passive</td>
<td>1.0</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>TKE</td>
<td>0.7</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Epsilon</td>
<td>0.7</td>
<td>$10^{-3}$</td>
</tr>
</tbody>
</table>

secondary breakup process. The no time counter algorithm [37] was adopted to account for droplet collisions. Frossling correlation was used for modeling droplet evaporation [38]. A dynamic drag model [39] and a turbulent dispersion model were used to model droplet drag and dispersion.

### 2.1.4 Numerical Parameters

The finite volume differencing scheme was used in the CONVERGE code to solve the governing equations with a transient implicit solver. The Pressure Implicit with Splitting of Operators (PISO) scheme was used for the pressure-velocity coupling. Under-relaxation was used to aid convergence for the transport equations. The convergence criteria is calculated based on a normalized error for each equation. The under-relaxation factors and convergence criteria used in this study are summarized for different equations in Table 2.1.

Time stepping is an important part of the solver set-up process. The transient solver with adaptive time stepping was used in the CFD code. The optimal time step at any given instance depends on the physics of the problem and a number of factors like spray
physics, species production and heat release. The CFL number \(u \frac{\Delta t}{\Delta x}\), Mach CFL number \(c \frac{\Delta t}{\Delta x}\) and diffusive CFL number \(v \frac{\Delta t}{\Delta x}\) are used to control the time-stepping in CONVERGE. Here \(u\) is the velocity, \(c\) is the speed of sound and \(v\) is the viscosity. Maximum limits are set for each of these CFL numbers along with an initial time step. After each iteration the CONVERGE code tries to increase the current time-step by 25 percent. If the convergence criteria mentioned is not achieved with the time-step or if it exceeds the CFL number limits then the time-step is reduced. For the spray simulation cases discussed in this study the these CFL number limits and convergence criteria were determined based on parametric studies. The maximum value of CFL number allowed in the simulation was restricted to 0.75.

When the spray model is active then the maximum time step is calculated by Equation 2.17 where \(\Delta x\) is the grid size and \(m_{\text{spray}}\) is an input parameter from the user which limits the maximum number of cells a parcel can travels in the given time step. Similarly, other parameters are used to control time stepping based on evaporation and temperature rise in a given cell.

\[
dt_{\text{spray}} = \min \left( \frac{\Delta x}{\text{parcel}_v} \right) \times m_{\text{spray}}
\]

where \(\text{parcel}_v\) is the velocity of a parcel the given cell. If droplet evaporation is active in a fluid domain then the maximum time step is given by Equation 2.18 where \(M_c\) is the total mass of the cell and \(M_{\text{evap}}\) is the mass evaporated from the previous time step, and \(dt_0\) is the previous time step. The user input parameter \(m_{\text{evap}}\) thus controls the maximum allowable evaporated mass in a single time step. Similarly, Equation 2.19 restricts the time step based on temperature rise in each cell where the input parameter is \(m_{\text{chem}}\). A maximum and minimum limit for time-steps have been specified. Table 2.2 summarizes
the input parameters for time step control used for the Spray A simulations.

\[ dt_{\text{evap}} = dt_0 \times \min \left( \frac{M_c}{M_{\text{evap}}} \right) \times m_{\text{evap}} \]  

(2.18)

\[ dt_{\text{chem}} = dt_0 \times \min \left( \frac{T}{\Delta T} \right) \times m_{\text{chem}} \]  

(2.19)

Table 2.2: Input parameters for adaptive time-step control.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m_{\text{spray}} )</td>
<td>0.5</td>
</tr>
<tr>
<td>( m_{\text{evap}} )</td>
<td>0.5</td>
</tr>
<tr>
<td>( m_{\text{chem}} )</td>
<td>0.5</td>
</tr>
<tr>
<td>Initial time-step</td>
<td>5e-7 s</td>
</tr>
<tr>
<td>Minimum time-step</td>
<td>1e-8 s</td>
</tr>
<tr>
<td>Maximum time-step</td>
<td>1e-6 s</td>
</tr>
</tbody>
</table>

2.2 Mesh

Meshing a 3D or 2D geometry for practical applications has always been a major hurdle in CFD simulations. The accuracy of the solution depends on the type of mesh and its resolution. High resolution grids are important to resolve flow features accurately. A fine mesh is required in regions where the gradients are higher. The traditional approach without adaptive meshing and fixed grids require an \textit{a priori} knowledge of the solution field and then refinement the grids in regions where the gradients in variables like temperature, velocity, species, etc. are higher. For turbulent unsteady problems these regions
move in space. As a result a large subsection of the mesh needs to be refined. The entire procedure would need to be repeated iteratively based on the solution to arrive at a grid independent solution. This is a brute force approach and in order to demonstrate grid convergence a very large mesh needs to be generated and solved.

Unsteady engine combustion simulations involve spray injection events coupled with moving boundaries. A fine mesh is required only for regions near the spray and a coarse mesh would suffice for the other regions. Fuel air mixing layers that are formed along the stoichiometric regions exhibit the most chemically reactive regions for non-premixed combustion. It is important to have higher mesh resolution in these regions to resolve the chemistry and flow accurately. Adaptive meshing is well suited for such problems and has a robust implementation in Converge for complex as well as moving geometries. The mesh refinement is changed at every time step depending on the solution at each time step as shown in Figure 2.3. In these plots the computational grids are in 3 dimension but the comparisons are made between the slices of $x - y$ plane along the center-line of the spray. The upper half of the domain represents the coarse mesh. The base grid size ($dx_{\text{base}}$) is the default size of the initial grid generated over the entire domain. This is set to 4 mm for the baseline mesh. Fixed embedding is a feature that allows the user to refine the grid selectively at certain places. In spray cases usually the region near the nozzle is refined using fixed embedding. The input parameter $\text{embed}_{\text{scale}}$ determines the size ($dx_{\text{embed}}$) of mesh near the embedded region and is given by Equation 2.20.

$$dx_{\text{embed}} = dx_{\text{base}} \times 2^{-\text{embed}_{\text{scale}}}$$  \hspace{1cm} (2.20)

The embedded scale was set to 4. The start of injection is at 0 ms. As the spray parcels penetrate the domain the mesh is automatically refined in the regions of spray. At 0.6
ms higher resolution grids are generated in the flame region.

The AMR algorithm in CONVERGE adds higher grid resolution at regions where the gradients of specified variables are highest. In this study the AMR was based on velocity and temperature fields. This combination can capture the spray as well as the fuel air mixing regions accurately. The input parameters $amr_{\text{embed}, \text{vel}, \text{scale}}$ and $amr_{\text{embed}, \text{temp}, \text{scale}}$ are used to control the minimum cell sizes generated in regions of high gradients. The mesh size is given by Equation 2.21

$$dx_{\text{embed}} = dx_{\text{base}} \times 2^{-amr_{\text{embed}, \text{vel}, \text{scale}}}$$  \hspace{1cm} (2.21)

For the baseline case these values are summarized in Table 2.3. These values will lead to a minimum cell size of 0.25 mm. For running a finer mesh for the same problem only the base grid size is changed. Thus, a base grid size of 2 mm will lead to a minimum grid size of 0.125 mm and 8 mm base grid size will lead to a mesh with smallest grid size of 0.5 mm. These grids are generated at runtime and a new mesh is generated at every time step based on the AMR settings and the solution of the problem.

Table 2.3: Input parameters for adaptive mesh refinement with baseline mesh (0.25mm min. cell size).

<table>
<thead>
<tr>
<th>AMR Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base grid</td>
<td>4 mm</td>
</tr>
<tr>
<td>Nozzle Embed Scale</td>
<td>4</td>
</tr>
<tr>
<td>Velocity AMR Embed Scale</td>
<td>4</td>
</tr>
<tr>
<td>Temperature AMR Embed Scale</td>
<td>4</td>
</tr>
<tr>
<td>Maximum Cell Count</td>
<td>0.8 million</td>
</tr>
</tbody>
</table>
Figure 2.3: Adaptive Mesh Refinement: Comparison between (a) coarse mesh (0.5mm smallest grid size) and (b) fine mesh (0.25mm smallest grid size) for Spray A conditions at different time-steps.
2.3 Reaction Mechanisms

In this study n-dodecane was used as the surrogate to model chemical kinetics. Two different skeletal mechanisms were considered and both were derived from a detailed mechanism consisting of 2115 species and 8157 reactions from Lawrence Livermore National Laboratory [40]. The 103 species reaction mechanism was obtained by applying the Directed Relation Graph (DRG) reduction technique together with expert knowledge (called DRGX) to the above-mentioned detailed mechanism by Lu and co-workers [29]. While this skeletal mechanism was observed to perform well in capturing ignition characteristics of n-dodecane, it was not able to capture the flame speed trends. Hence, certain reaction rates were tuned, and a few species and reactions were added, to match gas phase flame speed values in addition to homogeneous ignition delays. Due to these changes in reaction rates, a new n-dodecane with 106 species and 420 reactions was obtained by Luo et al. [41]. Zero dimension simulations were carried out using SENKIN [42] to compare the 2 reaction mechanisms. These simulations assume perfectly stirred reactor conditions for a given equivalence ratio. Figure 2.4 shows the ignition delay as a function of temperature for an equivalence ratio of 2. The ignition delay predictions are similar for the 700 K to 850 K range. The 106 species mechanism predicts higher ignition delays for higher temperature ranges above 850 K. The difference reduces for temperatures above 1100 K. The engine conditions simulated for spray A and single cylinder diesel engines are within the 800 K to 1200 K range.
2.4 High Performance Computing Resources

Detailed modeling approaches with highly resolved grids are important to develop predictive CFD models. However, they require large computational resources. CFD modeling capabilities are dictated by the availability of computational resources. Lower costs of High Performance Computing (HPC) technology has significantly enhanced the development of high fidelity models over the past two decades. The CONVERGE code was run on HPC clusters in a parallel environment. The simulations were run on two different clusters at Argonne National Laboratory. The ‘Blues’ cluster is a 310 node (Intel Sandy Bridge) machine with 4960 processors with QLogic QDR infiniband interconnect with a peak performance of 107.8 teraflops. The RANS Spray A simulations were run with 3 nodes (16 processors each), i.e., 48 parallel processors. The engine cases were run with a maximum of 8 nodes, i.e., 128 processors. The chemistry tabulation codes and the iterative steady strain solvers were run on this cluster with 4 nodes, i.e., 64 processors.
Each node has 64 GB of Random Access Memory which is shared between 16 processors. The memory available for each node is an important factor especially for tabulated combustion models and for large meshes. The tabulation and cell data are stored in memory during runtime. The Message Passing Interface implementation creates a copy of the arrays for each processor and stores them in the RAM for fast access. This can lead to memory issues for runs with large meshes. Codes were developed considering this memory bottleneck.

The ‘Fusion’ cluster is a relatively small machine with a peak performance of 30 teraflops, 320 nodes with 8 processors per node with Infiniband QDR interconnect. Each node shares 36 GB of RAM. This cluster was used to run the Spray A cases with 4 nodes i.e. 32 processors in parallel.

### 2.5 Conclusions

The implementation of the CONVERGE CFD code was discussed in this chapter. Detailed explanation of the modeling approaches, problem setup and grids was presented. The governing equations, turbulence models, spray models and chemistry mechanisms were discussed in detail. The availability of a high fidelity code with established modeling approaches provide a robust framework to establish baseline models, evaluation of current models and implement new combustion models. New codes can be developed for combustion modeling approaches and coupled easily with such established frameworks. It can also help in establishing frameworks for comparative study between different models. The codes developed in the proceeding sections are interfaced with the CONVERGE code.
Chapter 3

The Representative Interactive Flamelet Model

3.1 Introduction

The finite-rate chemistry combustion models have been used extensively to model reacting flows for a wide range of applications. These models assume that every cell in the domain as a perfectly stirred reactor. The chemical source terms are evaluated at Favre-averaged temperatures. The source terms are highly non-linear in temperature. Thus, evaluating the source terms with averaged temperatures could lead to significant errors in turbulent combustion flows. Thus, it is important for models to consider the effect of turbulence-chemistry interaction. The multi-flamelet Representative Interactive Flamelet (RIF) model [43,44] is used to account for the effects of turbulence-chemistry interaction (TCI) to model spray combustion under typical diesel engine conditions. The RIF model calculates the species mass fraction based on the mixture fraction fields and scalar dissipation rates provided by the Computational Fluid Dynamics solver. A time-dependent
RNG turbulence model is used in conjunction with a grid-converged discrete phase model for the liquid phase. The minimum number of flamelets required is determined to sufficiently represent the large variation of stoichiometric scalar dissipation rates in the domain. Different forms of the presumed scalar probability density functions (PDFs) were also examined. The modeling results are then compared with the experimental data at different ambient temperatures, ambient O_2 concentrations, ambient densities, and injection pressures. The effects of different chemical kinetic mechanisms (103-species and 106-species skeletal mechanisms) are also studied to further understand the performance of the model. Overall, the RIF model is observed to capture the measured ignition delay and flame lift-off length very well, especially under certain conditions characterized by low ambient temperatures, densities, and oxygen concentrations. The need for initializing multiple flamelets is highlighted in order to obtain simulation results devoid of modeling artifacts. Overall, the efficacy of using an advanced turbulent combustion model is demonstrated. The same modeling framework is then applied towards modeling a single cylinder diesel engine. Parametric variations show exactly the same type of trends that were observed with the Spray A cases and the simulation results match well with the reported experimental data.

3.1.1 Governing Equations

The RIF model was proposed and derived by Pitsch et. al. [45], which was based on the laminar flamelet concept by Peters [46] and [47]. The RIF combustion model calculates the species mass fraction based on the knowledge of Favre averaged mixture fraction (\( \tilde{Z} \)) and mixture fraction variance (\( \tilde{Z}^2 \)) in the flow field. Therefore, two additional transport equations for and are solved within the CFD solver:
\[ \frac{\partial (\bar{p}\bar{Z})}{\partial t} + \frac{\partial (\bar{p}\bar{u}_l\bar{Z})}{\partial x_l} = \frac{\partial (\bar{p}u''_l\bar{Z}'')}{\partial x_l} \]  

(3.1)

where

\[ u''_l\bar{Z}'' = -D_l \frac{\partial \bar{Z}}{\partial x_l} \]  

(3.2)

\[ \frac{\partial (\bar{p}\bar{Z}^2)}{\partial t} + \frac{\partial (\bar{p}\bar{u}_l\bar{Z}^2)}{\partial x_l} = -\frac{\partial (\bar{p}u''_l\bar{Z}'')}{\partial x_l} - 2(\bar{p}u''_l\bar{Z}'') \frac{\partial \bar{Z}}{\partial x_l} - \bar{p}\dot{\chi} \]  

(3.3)

The scalar dissipation rate is modeled as \( \dot{\chi} = c_x \frac{\varepsilon k}{Z^2} \) where \( c_x \) is a mixing constant, \( k \) is the turbulent kinetic energy and \( \varepsilon \) is the dissipation rate obtained from the turbulence model. The value of \( c_x \) was set equal to 2 for all cases. The flamelet equations 3.4 and 3.5 were derived from the species conservation equation by applying a coordinate transformation to the mixture fraction (\( Z \)) space [46].

\[ \rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i \]  

(3.4)

\[ \rho \frac{\partial T}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \rho \frac{\chi}{2C_p} \left[ \sum \left( C_{pi} \frac{\partial Y_i}{L e_i \partial Z} + \frac{\partial C_{pi}}{\partial Z} \right) \right] \frac{\partial T}{\partial Z} = \frac{1}{C_p} \left( \frac{\partial P}{\partial t} - \sum \dot{\omega}_i h_i \right) \]  

(3.5)

In order to solve these set of partial differential equations 3.4 and 3.5, the scalar dissipation rate \( \chi \) should be converted from a function of physical space to a function of mixture fraction. The following equation 3.6 derived in [46] was used to perform the transformation:

\[ \chi(Z) = \chi_{st} \frac{f(Z)}{f(Z_{st})} \]  

(3.6)
where
\[ f(Z) = \exp[-2(\text{erfc}^{-1}(2Z))]. \quad (3.7) \]

\( \tilde{\chi}_{st} \) is the domain averaged scalar dissipation rate conditional over the stoichiometric mixture fraction and erfc is the error function. In order to construct the flamelet library for the entire CFD domain, the average value is calculated using Equation 3.8

\[ \tilde{\chi}_{st} = \frac{\int_v \rho \tilde{\chi}_{st} \frac{3}{2} \tilde{P}(Z_{st})}{\int_v \rho \tilde{\chi}_{st} \frac{1}{2} \tilde{P}(Z_{st})} \quad (3.8) \]

where
\[ \tilde{\chi}_{st} = \frac{f(Z_{st})}{\int_0^1 f(Z)P(Z)dZ} \quad (3.9) \]

\( v \) is the volume of the entire computational domain and \( P() \) is the probability density function (PDF). Solving the flamelet equations 3.4 and 3.5 gives the species mass fraction \( Y_i \) as a function of \( Z \). A beta PDF distribution of the mixture fraction as shown in Equation 3.10 is assumed to calculate the mass fraction \( Y_i \) in each cell with Equation 3.11. The presumed shape of beta PDF, \( P(Z; x, t) \), was also used in the previous equation 3.8.

\[ P(Z; x, t) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1}}{\Gamma(\alpha)\Gamma(\beta)}\Gamma(\alpha + \beta) \quad (3.10) \]

\[ \tilde{Y}_i(x, t) = \int_0^1 Y_i(Z, t)P(Z; x, t)dZ \quad (3.11) \]

Instead of using just one flamelet library, multiple flamelet libraries were used with each flamelet accounting for a certain fraction of the injected fuel. A mass-weighted fraction of the fuel that are being injected were tracked using marker Equation 3.12,
which were solved for each flamelet generated:

$$\frac{\partial (\bar{\rho} \bar{Z}_l)}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_l \bar{Z}_l)}{\partial x_l} = -\frac{\partial (\bar{\rho} \bar{u}_l \bar{Z}_l^\prime)}{\partial (x_l)}$$ \hspace{1cm} (3.12)

These markers must also satisfy 3.13

$$\bar{Z} = \sum_{1}^{n} Z_l$$ \hspace{1cm} (3.13)

where \( n \) = number of flamelets

The averaged value of stoichiometric scalar dissipation rate for each flamelet is calculated as:

$$\hat{\chi}_{st}(l) = \hat{\chi}_{st} = \frac{\int_{V} \bar{Z}_l \bar{\rho} \bar{\chi}_{st}^{3/2} \bar{P}(Z_{st})}{\int_{V} \bar{Z}_l \bar{\rho} \bar{\chi}_{st}^{1/2} \bar{P}(Z_{st})}$$ \hspace{1cm} (3.14)

### 3.2 Modeling Spray Flames with RIF

The focus of this study is the reacting cases at different ambient conditions, including variations of ambient temperature, ambient oxygen concentration, injection pressure, and ambient density. The grid convergences for the RIF model was first studied, followed by the selection of number of flamelets. After establishing the baseline setup, comprehensive studies of reacting cases are presented.

#### 3.2.1 Non-reacting Cases

Fuel-air mixing plays an influential role in spray combustion problems. The spray breakup and evaporation processes are important factors influencing ignition and flame stabilization. The Lagrangian-Eulerian spray model is validated in this section against available experimental data for non-reacting cases. The non-reacting Spray A case with 900 K am-
Figure 3.1: Temporal evolution of liquid penetration and vapor penetration for non-reacting Spray A case.

Ambient temperature, 22.8 kg/m$^3$ ambient density with 150 MPa injection was simulated in the CONEVRGE code for an injection duration of 1.5 ms. Liquid penetration is defined as the axial location from the nozzle that encompasses 97 percent of the injected mass at any given time instant. Vapor penetration is defined as the farthest downstream location of 0.05 percent fuel mass fraction contour.

Figure 3.1 shows the predicted and experimentally measured liquid and vapor penetration for the non-reacting Spray A case. The liquid penetration increases with time at the start of injection. It reaches a quasi-steady state at 0.1 ms, and then remains constant up to the end of injection at 1.5 ms. The liquid penetration predicted by the spray model
shows a similar trend and the predictions are close to the experimental values with slight under-prediction. Initially the vapor penetration increases rapidly and then increase at a lower rate. This trend is also captured by the simulation. The simulations initially over-predict the vapor penetration and after 0.5 ms of injection show slight over-prediction. The spray model captures the spray break-up and mixing process for the Spray A setup.

### 3.2.2 Grid Convergence

Three meshes with different values of minimum grid size i.e., 0.5 mm, 0.25 mm and 0.125 mm were studied to assess the grid convergence for the RIF combustion model. These minimum grid sizes were obtained from a base mesh size of 1 mm together with different levels of AMR and embedding. This resulted in a peak cell count of about 630,000 for the finest resolution of 0.125 mm at 1.5 ms. The ignition delay and flame lift-off length are the metrics to evaluate the results from different meshes. The ignition delay was calculated based on the maximum temperature in the domain and defined as the time from start of injection (SOI) to the instant of the maximum temperature rise. The lift-off length in experiments was defined based on OH chemiluminescence; however, since OH* was absent from the simulations, the lift-off length was defined as the distance from the injector to the 14 percent maximum ground state OH at steady state. These two definitions are the recommendations from ECN2 workshop (Engine Combustion Network (2013) [1]).

Figure 3.2 shows the temporal variation of lift-off length for the RIF model on different grids compared to the experimental data. The difference of the predictions between the minimum grid size of 0.25 mm and 0.125 mm is very subtle. However, the computational cost increases significantly from mesh size of 0.25 mm (2160 CPU hours) to that of 0.125 mm (8544 CPU hours). The minimum grid size of 0.25 mm is chosen for the baseline
mesh considering the balance of accuracy and computational cost. One may argue the
difference for the RIF results at the earlier timing is relatively large between the mesh
size 0.25 mm and 0.125 mm. The 0.25 mm mesh was run on This is not going to affect
the lift-off length predictions significantly since the lift-off length is an average value over
quasi-steady state where the difference for these two meshes is rather small (1 mm).
Based on these results the 0.25 mm mesh is chosen as the baseline for calculations.

### 3.2.3 Effect of Multiple Flamelets

As discussed earlier, one of the shortcomings of the RIF model is that the domain averaged
scalar dissipation rate $\chi_{st}$ cannot capture the effects of the varying scalar dissipation rate
conditional on stoichiometric mixture fraction, which may lead to inaccurate predictions.
Initially the RIF model was run on the baseline case with 1 flamelet. The ignition delay
was observed to be 1.6 ms compared to the experimental data of 0.44 ms. In order to
better account for the variation of $\chi_{st}$ on the RIF model the simulations were run with increased number of flamelets as reported in Figure 3.3. Figure 3.3 shows the temporal lift-off length with different number of flamelets compared to the experiments. With 2 flamelets the lift-off length shows incorrect trends compared to experiments i.e., it keeps increasing with time. As the number of flamelets was increased to 6 the lift-off length trends improve but the quantitative values show an oscillatory behaviour. The amplitude of oscillation decreases with increased number of flamelets and finally with 20 flamelets, the oscillations disappear completely and the lift-off length is fairly stable. The predictions of ignition delays and lift-off lengths with respect to the number of flamelets are shown in Figure 3.4. As one can see, the estimations for both the lift-off length and ignition delay vary by a large amount when increasing from 1 to 16 flamelets; however, with more than 20 flamelets the solutions do not change significantly. The lift-off length for 40 and 60 flamelets are identical. Hence convergence with respect to the number of flamelets was observed.
Figure 3.4: Ignition delay and lift-off lengths for different number of flamelets.

The qualitative results for auto-ignition and flame stabilization for different flamelets are shown in Figure 3.5. It is observed that the single flamelet case ignites at 1.6 ms and does not predict any lift-off behaviour. The 20 and 60 flamelet cases predict identical contours and there is no difference in the qualitative results as well.

Figure 3.6 shows the temporal evolution of the domain averaged and every individual flamelets stoichiometric scalar dissipation rate for the case with 30 flamelets. It can be seen that the domain average stoichiometric scalar dissipation rate increases and then rapidly decreases to a smaller value. The regions near the spray are generally characterized by higher values of scalar dissipation rate. As the fuel injection starts the stoichiometric regions are formed near the spray region and they tend to move far away from the spray as time progresses. This causes a reduction in the average value of the stoichiometric scalar dissipation rate. Similar behaviour is observed for the individual flamelets as well. As new flamelets are initialized they account for the fuel closer to the injection region and then with time they move away from the spray towards regions of lower scalar dissipation
Figure 3.5: Temperature contour plots for cases with different number of flamelets.
Figure 3.6: Stoichiometric Scalar dissipation rate evolution for different flamelets.

rate. This occurs successively for each individual flamelet.

This oscillatory behaviour of flame lift-off length (Figure 3.3) can be explained from Figure 3.7, which shows the predictions of heat release rate for different number of flamelets with the RIF model. The heat release rate with 2 flamelets increases after the ignition delay and has 2 bumps. With increase in the number of flamelets the amplitude of the oscillations decreases and the frequency goes on increasing with time. Finally, when the number of flamelets is sufficient, the oscillations die down and a steady heat release curve is observed.

For the single flamelet case, a single set of flamelet equations are used to account for chemistry in the whole domain. These flamelet equations use a stoichiometric scalar dissipation rate which is calculated as an average over the whole domain. This single averaged value is not representative of the large spatial variation in the stoichiometric scalar dissipation rate for the entire domain as shown in Figure 3.8. It shows the scalar dissipation rate conditional on stoichiometric mixture fraction contour as a function of
Figure 3.7: Heat Release Rates for multiple flamelets.
the axial distance from the noxxle.

To further understand this, one may consider the case with 2 flamelets initialized far apart. Once the first flamelet ignites, all fuel that has been added to the domain will be accounted for by this burnt flamelet, which will lead to the increase in the heat release rate. The heat release rate will be brought down when a new flamelet is initialized and the new fuel added to the domain will be accounted by this unburnt flamelet. When this newly generated flamelet reaches burnt state again, all fuel being accounted for by this flamelet will spontaneously ignite. This will result in another bump in the HRR curve. With an increase in total number of flamelets each flamelet will account for a lower amount of fuel and they will ignite sequentially as per their local scalar dissipation rates. Thus, these oscillations will have a lower magnitude and become more frequent. A large
The above paragraph clearly demonstrates the need for the RIF model to have a sufficient number of flamelets to account for the large variation of the scalar dissipation rate. In Figure 3.4 the lift-off lengths and ignition delays from 60, 30 and 20 flamelets are almost identical, which indicates that 20 flamelets are sufficient for the baseline RIF cases at 900 K ambient condition. However, Figure 3.4 suggests that 30 flamelets provide a better estimate for the heat release rate. Since our focus is on the predictions of lift-off length and ignition delay in this study, 20 flamelets were adopted for the baseline case. Increasing the number of flamelets results in higher computational cost as shown in Figure 3.9. These simulations were run for the same grids with different number of flamelets on 32 processors.

From the above observations it seems that the number of flamelets should be dependent on the amount of fuel being accounted by each flamelet. However, simulations
under some other conditions show that this estimation is not sufficient. A higher ambient temperature of 1200 K with 1.5 ms duration of injection was simulated with 20 and 40 flamelets as shown in Figure 3.10. One can notice from Figure 3.10 that the lift-off length has oscillatory behaviour with 20 flamelets. This was not observed for the 900 K baseline case with the same number of flamelets. The reason is that the 1200 K case has a shorter lift-off length and a further upstream lift-off location. Thus, the value of $\chi_{st}$ around stabilization location is much higher, as presented in Figure 3.8. This indicates that higher $\chi_{st}$ around the flame stabilization location would require more flamelets to account for the larger variation of $\chi_{st}$. It is also interesting to note that $\chi_{st}$ does not vary much for the two ambient temperature cases.

Figure 3.10: Lift-off lengths at 1200 K.
### 3.2.4 Presumed Form of Scalar PDFs

A presumed form of scalar PDFs was used to calculate the species mass fraction in each cell with the solution from the flamelet equations. This PDF describes the statistical variances occurring in the turbulent flow. Typically beta PDFs are used for turbulent combustion problems. The role played by the form of presumed PDF is studied in detail in this section. Three different schemes were investigated viz. delta, beta and Gaussian PDF. In order to implement a delta PDF the following procedure was followed. The flamelet equations were solved for each flamelet to yield the species mass fractions as functions of $Z$. The mixture fraction is known for each cell in the CFD domain. This mean value of $Z$ was mapped directly to the flamelet solution to calculate the species mass fraction. This process eliminates the role of the mixture fraction variance and effect of turbulent fluctuations and is same as having a delta PDF.

Figure 3.11 and Figure 3.12 show the qualitative differences between the results obtained by delta, beta and Gaussian PDFs. These simulations were set up with the 103 species mechanism and 20 flamelets. The delta PDF which neglects the variances and the integration process predicts a higher temperature and also a higher gradient in OH mass fraction. The peak values of OH are also higher. It can be observed in Figure 3.11(b) that the beta PDF integration results in reduction of temperature and smearing of the gradients. A similar trend is also observed with the OH distribution with beta PDF in Figure 3.12(b). The beta PDF integration tends to smear the gradients and also results in a reduction of peak values of temperature and OH species mass fraction.

The clipped Gaussian PDF results match the results very closely from beta PDF with respect to the temperature distribution as shown in Figure 3.13. Both PDFs were able to capture the lift-off lengths accurately. The ignition delay predicted by the beta PDF was
Figure 3.11: Temperature contour comparisons for different presumed PDF functions: (a) delta PDF, (b) beta PDF, and (c) Gaussian PDF.

Figure 3.12: OH contour comparisons for different presumed PDF functions: (a) delta PDF, (b) beta PDF, and (c) Gaussian PDF.
0.55ms and that from Gaussian PDF was 0.575ms. The experimental value reported was 0.44 msec. However, the Gaussian PDF predicts higher values of OH with a thin region of high concentration of OH as shown in Figure 3.13. Overall, both the PDF integration schemes were able to capture the ignition delays and lift-off lengths. The beta PDF was used for the rest of the study.

Figure 3.13 shows quantitative comparisons of the different PDF integration methods across a sweep of temperatures. Overall, it is observed that the beta PDF as well as Gaussian PDF predict very similar ignition delays; however, the predictions of lift-off lengths from the Gaussian PDF are slightly closer to the experimental values.

3.2.5 Temperature Sweep

Figure 3.14 shows the quantitative comparison of ignition delay and lift-off length for both the well-mixed and RIF models compared to the experimental results. Two different chemistry mechanisms, the 103 species ndodecane mechanism with 370 reactions and 106 species with 420 reactions were used for modeling chemical kinetics. The predictions of ignition delay from the two combustion models with respect to the two chemistry mechanisms are reported in Figure 3.14. With the 106 species reaction mechanism, the RIF model predicts much better ignition delays. The sensitivity with respect to different ambient temperatures is also better captured compared to the well-mixed model across the entire temperature range. One may also notice that the over-predictions from both combustion models across the entire temperature range, which was systematically investigated by Pei et al. [10]. In their study, both the effect of minor species, such as OH and NO, and the chemistry mechanism itself were studied and it was concluded that the mechanism itself was the reason for the over-predictions compared to the experiments at
Figure 3.13: Ignition delay and lift-off lengths for different ambient temperature conditions with delta PDF, beta PDF and Gaussian PDF.
these ambient conditions. Similar over-predictions were also observed for the 103 species mechanism except that similar or better predictions were obtained at the higher ambient temperatures of 1000 and 1100 K for the well-mixed model. Comparing the two mechanisms for the well-mixed model, one may notice similar predictions for the lower ambient temperature conditions and much better estimations for the 103 species mechanism at the higher ambient temperature conditions. However, this is not observed for the RIF model which predicts similar ignition delays across the ambient temperature conditions considered here.

For the two mechanisms considered, the predictions from the RIF model for lift-off are much better than those of well-mixed model at the lower ambient conditions. Predictions are quite similar for the higher ambient temperature conditions for the 106 species mechanism for the two combustion models. It is interesting to note that the RIF model is less sensitive to the reaction mechanisms used.

### 3.2.6 Ambient Oxygen Sweep

The effect of ambient oxygen concentrations were examined for both the well-mixed and RIF models together with the two chemistry mechanisms. The baseline case with 900 K ambient temperature was used with the variations of the ambient oxygen concentration of 13, 15 and 21 percent. The predictions of the ignition delay are reported in Figure 3.15. As one may notice, the well-mixed models over-predicts the ignition delay compared to the measurements for both mechanisms at different ambient oxygen conditions. However, the predictions are better with the 106 species mechanism and it also captures the sensitivity with respect to the variations of the ambient oxygen concentration. The 103 species mechanism over-predicts the sensitivity for the well-mixed model. The RIF model
Figure 3.14: Ignition delay and lift-off lengths for different ambient temperature conditions.
predicts the ignition delays significantly better than the well-mixed model for different ambient oxygen concentrations for both the mechanisms. It is noted that the predictions at 21 percent oxygen condition are very accurate for both mechanisms. However, at lower ambient oxygen concentrations simulations with both RIF and well-mixed models were found to over-predict ignition delays. The values predicted by the RIF model were significantly better than the well-mixed model.

Lift-off length calculations are also presented in Figure 3.15. The results from both mechanisms over-predict the sensitivity with respect to different ambient oxygen conditions for the well-mixed model although relatively good estimations were found for the 21 percent oxygen condition. However, the RIF model predicts better sensitivity for both mechanisms with more accurate estimations at lower oxygen concentration of 13 percent and some over predictions at 15 and 21 percent ambient oxygen conditions. The less sensitivity to the chemistry mechanisms was again observed for the ambient oxygen conditions studied here.

### 3.2.7 Injection Pressure Sweep

The variations of injection pressure were studied by performing simulations at 50, 100, and 150 MPa at an ambient temperature of 900 K. Figure 3.16 reports the ignition delay predictions for both the well-mixed and RIF combustion models and the two different chemical kinetic mechanisms. The measurements were found to decrease with increase in the injection pressures, which was due to the better mixture formation at higher injection pressures. It can be seen that the well-mixed model predicts inaccurate trends for the sensitivity with respect to the variation of injection pressure for both the mechanisms. The RIF model better predicts the sensitivity although marginal over-predictions are found.
Figure 3.15: Ignition delay and lift-off lengths for different ambient oxygen concentrations.
for all injection pressures for both mechanisms. Similar predictions of lift-off lengths are reported, the RIF model predicts correct sensitivity with respect to the variation of injection pressure and more accurate results compared to the experiments for both mechanisms. Again, at different injection pressures over-prediction of the sensitivity to oxygen concentration was observed for the well-mixed model. Consistent with previous findings, the RIF model is less sensitive to the reaction mechanisms used for the conditions considered in this section.

3.2.8 Ambient Density Sweep

The effect of change in ambient density (from baseline condition of 22.8 kg/m³ to 15.7 kg/m³) at 900 K is studied in this section. The predictions of ignition delay and lift-off length are reported in Figure 3.17 and overall similar observations were found. It can be seen that all the simulations over-predict the measurements with RIF better capturing the sensitivity with respect to the variation of ambient density than the well-mixed model. For the lift-off length predictions reported, the RIF model predicts better sensitivity and more accurate results than the well-mixed model compared to the measurements. Less sensitivity of the RIF model to the chemistry mechanism is found again for the conditions studied.

3.2.9 Qualitative Difference Between RIF and Well-Mixed Model

Figure 3.18 shows the qualitative difference in the flame structure between the two models at 1ms after start of injection. These results are for the 900 K ambient temperature case with the 106 species and 420 reactions. The white line contour on the OH plot and black line on the temperature plots show the 14 percent max. OH line i.e. the lift-off contour.
Figure 3.16: Ignition delay and lift-off lengths for different injection pressures.
Figure 3.17: Ignition delay and lift-off for different ambient densities.
Figure 3.18: Qualitative results from RIF and well-mixed model: (a) OH mass fraction contour (b) Temperature contour.

The well-mixed model predicts higher temperatures and OH as compared to the RIF model. The flame structure is also different compared to RIF. The well-mixed model predicts a horse-shoe shaped OH contour with higher gradients. The RIF model on the other hand predicts smeared OH and temperature profiles. The lift-off length predicted by the RIF model is lower compared to that predicted by the well mixed model. Similar comparison at the 13 percent ambient oxygen concentration is shown in Figure 3.19. The RIF model predicts higher temperatures and lift-off lengths. Well-mixed model predicts higher gradients in temperature and the RIF model predicts a smeared profile. Also the RIF model tends to predict a broader flame.

3.3 Diesel Engine Modeling with RIF Model

The previous sections demonstrate the implementation and validation of the RIF model for spray flame applications. An approach for improving the numerical approach with the RIF model was presented and then applied for spray flames. This section will further evaluate the performance of RIF model in a single cylinder diesel engine. The effect of the
Figure 3.19: Qualitative results from RIF and well-mixed model, temperature contour for 13 percent ambient O\textsubscript{2} conditions.
number of flamelets was investigated using the same method discussed in the previous section.

The experimental setup consisted of a single cylinder turbocharged research engine. The Caterpillar Hydraulic Electronic Unit Injector (HEUI) 315B injector with 6 holes was used in this engine. More details regarding the injector nozzle geometry can be found in [48]. The other engine specifications are listed in Table 3.1. The engine speed was fixed at a constant value of 1500 rpm. The oil rail pressure in the HEUI injection system was set at 170 bar which corresponds to a peak injection pressure of 1122 bar. The cylinder pressure was measured using a piezoelectric water cooled pressure transducer.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
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</thead>
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<td>Engine Model</td>
<td>Caterpillar 3410E</td>
</tr>
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<tr>
<td>Stroke</td>
<td>165.1 mm</td>
</tr>
<tr>
<td>Displacement</td>
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<tr>
<td>Compression Ratio</td>
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</tr>
<tr>
<td>Combustion Air System</td>
<td>Simulated turbocharger and air-to-air aftercooler</td>
</tr>
<tr>
<td>Combustion air system</td>
<td>HEUI 315B, six-hole tip</td>
</tr>
</tbody>
</table>

### 3.3.1 Computational Model

The 3D geometry consists of the piston bowl, cylinder liner and cylinder head rendered as per the actual engine. A 60 degree sector was generated for the closed cycle CFD simulation. Figure 3.21 shows the geometry along with the boundaries. The piston bowl was
Figure 3.20: Adaptive Meshing for Engine Cases.
Figure 3.21: Single cylinder engine geometry with sector mesh.

specified as a moving boundary in CONVERGE with no-slip wall boundary conditions. The movement of the piston was enforced by the specified RPM in the CONVERGE code. Symmetry boundary condition was specified at the wedge boundaries as shown in Figure 3.21. The engine simulations were initialized at intake valve closure (IVC) with uniform temperature, pressure and species mass fraction. The 106 species and 420 reactions n-dodecane mechanism was used. Figure 3.20 shows the grids generated at runtime. The base grid size was set to 1.4 mm and the adaptive embedding resulted in a minimum grid size of 0.35 mm. Fixed embedding was activated for piston and cylinder head boundaries. The simulations were performed for a closed cycle where the SOI was at -7.71 degrees of crank angle. The rate of injection profile was reproduced from the experiments by Ramirez et al [48]. The flamelets were initialized sequentially from the start of fuel injection to the end of injection.
3.3.2 Results with Multiple Flamelets

Figure 3.22 shows the heat release rates predicted by the RIF model with different numbers of flamelets. Non-physical oscillations in the heat release rates can be observed for 20 and 40 flamelets even though the result for 1 flamelet is rather smooth. This behaviour was also observed in the Spray A cases with less than 20 flamelets. Each flamelet ignites individually depending on the stoichiometric scalar dissipation rate. With the increase in the number of flamelets each flamelet will account for a smaller portion of the fuel. Each flamelet will ignite, depending on the value of its stoichiometric scalar dissipation rate. The amplitude of oscillation becomes smaller with increased numbers of flamelets. The result from 1 flamelet is smooth because it does not have multiple flamelets igniting sequentially. It also can be noticed that the results from the 64 and 80 flamelets cases are almost identical, which indicates the convergence with respect to number of flamelets was achieved. 64 flamelets are sufficient to account for the spatial variation of the stoichiometric scalar dissipation rates and to predict the heat release rate. Figure 3.23 shows the
pressure traces for different number of flamelets. It can be seen that the single flamelet case predicts a higher peak pressure in the cylinder compared to the multiple flamelet cases. This is because all the fuel being injected into the cylinder is accounted for by a single flamelet. When this flamelet ignites, most of the fuel in the chamber will ignite, leading to higher heat release rates and higher peak pressures. By increasing the number of flamelets, each flamelet ignites independently depending on the local conditions leading to slightly lower peak pressures in the cylinder. The pressure traces for the 64 and 80 flamelet cases are almost the same, which indicates that 64 flamelets is sufficient to solve the reactive flow field. In these simulations all the flamelets were initialized at equal time intervals from the SOI.
3.3.3 Qualitative Results

The effect of number of flamelets on engine simulations with respect to pollutant formation and flame lift-off are discussed in this section. Figure 3.24 shows the temperature contour plots from Top Dead Centre (TDC) to 50 degrees after TDC. The spray injection starts at -7 crank angle degrees (CAD). An ignited flame is seen at TDC for both the cases before the spray plume has hit the bottom of the engine bowl. The flame shape predicted by the 80 flamelet case differs from the single flamelet case. The single flamelet case predicts high temperature regions in the near nozzle region. A lifted flame structure is predicted by the RIF model with 80 flamelets. Figure 3.25 shows the OH contours at 10 CAD after TDC along with the lift-off iso-contour. It clearly shows that the single flamelet case does not predict a lifted flame. A single flamelet accounts for the entire chemistry of the combustion chamber. When this flamelet reaches an ignited state any fuel in the computational domain will ignite. With the presence of multiple flamelets each flamelet will account for a certain portion of the fuel and ignite independently as per the local scalar dissipation rate conditions. The ECN Spray A cases also showed that single flamelet simulations do not predict lifted flames. These factors influence prediction of pollutants.

Figure 3.26 shows the qualitative difference in pollutant formation for different number of flamelets. The single flamelet case predicts higher concentrations of CO especially in the near nozzle region. Simulations with 80 flamelets predict CO formation in the region downstream of the spray. The NOx predictions show a similar trend with the single flamelet case predicting higher NO concentrations in the near nozzle regions.
Figure 3.24: Temperature contour plots for single cylinder diesel engine simulations with single and 80 flamelets at different crank angle degrees.

Figure 3.25: Temperature contour plots for single cylinder diesel engine simulations with 1 and 80 flamelets at different crank angle degrees.
Figure 3.26: CO and NOx mass fraction contour plots for single cylinder diesel engine simulations with 1 and 80 flamelets.


3.4 Conclusions

The RIF model with multiple flamelets was used to investigate the effect of turbulent chemistry interactions in spray flames under diesel engine conditions. The model with 2 different reaction mechanisms were validated against the experimental data from Spray A across a wide range of conditions. The RIF model was able to capture auto-ignition and flame lift-off across a wide range of conditions. The need for multiple flamelets to account for large spatial variations in scalar dissipation rate was demonstrated and a detailed analysis on the effect of number of flamelets on the results was presented. The importance of a RIF calculation to demonstrate the convergence with respect to the number of flamelets is highlighted and the minimum number of flamelets required was studied to accurately predict the ignition delay, lift-off length, and heat release rates under different ambient conditions. The model was applied to a single cylinder diesel engine and the results closely matched the experimental pressure trace. The main conclusions are noted below:

1. Sufficient numbers of flamelets are needed to account for the large variation of scalar dissipation rate under different conditions considered in the study. Heat release rates can be used as a metric to verify the sufficiency of flamelets. The same pattern was observed for the constant volume spray flame as well as the single cylinder diesel engine.

2. The RIF model predicts a wider and more distributed flame structure with lower temperatures and OH concentrations than the well-mixed model.

3. Quantitative data for OH concentrations from experiments can shed further light on whether the RIF or well-mixed distributions are more accurate.

The main essence of the RIF model is to use an online flamelet library for each flamelet. Each flamelet evolves in time and the stoichiometric scalar dissipation rate
changes temporally. The implementation of an online unsteady library thus enables the model to account for the unsteady or the “history” of each flamelet. However, this comes at an added computational cost. The flamelet equations need to be solved for each flamelet at each time step followed by the PDF integration process in each cell. This makes the RIF model computationally expensive for practical cases like diesel engines. As shown in the previous sections a very large number of flamelets are required to get converged solutions for practical problems involving spray flames. This motivates us to study flamelet models in detail and develop computation strategies which are faster and scalable for large problems.
4.1 Introduction

The need to have adequate number of species in a reaction mechanism has been pointed out in a number of combustion simulations. The accurate modeling of the unsteady chemistry is important for capturing the ignition process as well as flame stabilization and lift-off characteristics. Chemistry mechanisms of real hydrocarbon fuels consist of hundreds of species and thousands of reactions. This leads to a large computational overhead for combustion CFD simulations. The finite-rate combustion model with a transport equation solved for each species is the basic model and has been widely used by many researchers. However, this method necessitates the solution of a transport equation for each species. The chemical source term in this transport equation is usually evaluated with averaged values which can be a source of error for highly turbulent flows. Computational cost increases drastically with the number of species. This makes RANS and LES simulations of practical applications with large meshes computationally prohibitive. The previous sections implemented chemistry mechanisms with hundreds of species and
reactions over two different combustion models, RIF and the finite-rate chemistry model. The RIF model uses multiple flamelets which are solved at run time followed by a presumed PDF approach to account for turbulence-chemistry interaction. This entire process is computationally expensive. Moreover a large number of flamelets are required to get accurate results. This has led to the implementation of many tabulated flamelet models. The flamelet equations are solved before runtime for a wide range of parameters and a library is generated where the species mass fractions are tabulated. The mixture fraction (Z) transport equations are solved at run time and species are interpolated based on mixture fraction.

The flamelet concept was successful in decoupling the chemistry from the fluid flow. The turbulent flame is viewed as a collection of different laminar flamelets. Flamelets express the chemistry and species mass fraction as a function of mixture fraction. The mixture fractions can be calculated by a transport equation in the CFD solver. The mapping of species from the mixture fraction space to physical space finally achieves the indirect coupling of the chemistry and fluid flow. This greatly reduces the stiffness of the system and only one equation for the mixture fraction needs to be solved. This concept has been used by an entire family of flamelet models with a wide diversity of implementation for capturing the different effects. These flamelet models can be coupled with presumed PDF functions to account for turbulence-chemistry interactions.

A chemical database can be created before runtime and then a look up scheme can be used to read values from this dataset. This reduces the computational effort significantly. The Flamelet Generated Manifold [49] and Flamelet Progress Variable [50] are some examples of tabulated combustion models which have been used widely for simulating a range of combustion problems in RANS as well as LES simulations. A number of flamelet models have been used to simulate diesel sprays. Ayyapureddi et al. [51] used the FGM
model with RANS to simulate the Sandia Spray A. Bekdemir et. al. used the FGM model within a Large Eddy Simulation to model Spray H. Tilou et. al. [52] used approximated diffusion flame and homogeneous reactor tabulated combustion models to model a diesel spray injection in LES simulations. Ameen et.al. [53] used a UFPV combustion model in RANS and LES to simulate diesel spray combustion and compared the results.

In all these tabulated combustion models progress variables have been used to parameterize the flamelets and introduce the unsteady character of the flamelets. This requires solving progress variable transport equations, which have unclosed source terms. The entire chemistry pathway is characterized only by the evolution of the species that are used to define the progress variable. The definition of the progress variable is not fixed and can influence results. The aim of the work in this chapter is to develop a combustion model which tabulates the chemistry without having to use progress variables. The idea is to use the framework of the Eulerian Particle Flamelet Model (multi flamelet RIF) with multiple flamelets. Each flamelet has its own characteristic time scale. The flamelets are tabulated with time as one of the parameters/dimensions of the tabulation scheme. Thus, the tabulation effort was aimed at reducing the computational cost for such detailed simulations using novel techniques.

4.2 Chemistry Tabulation

4.2.1 Tabulation Structure

The following schematic in Figure 4.1 shows the working of a flamelet model. The implementation of the new tabulated model was based on a similar structure. The following equations are solved by the CFD solver: Continuity, Momentum, Energy, Mixture frac-
tion and Mixture fraction variance. Each iteration of the CFD solver gives the mixture fraction and enthalpy values for each cell. The flamelet equations are then solved for the given time step and this returns the species mass fractions as a function of mixture fraction $Y(Z)$ for each flamelet. A beta PDF is then constructed using the mean and variance ($Z^2$) of the mass fractions. This PDF is multiplied by the species function $Y(Z)$ and then integrated to give the final species mass fraction. Once the species mass fractions are calculated then the temperatures can be back-calculated from the enthalpy. This process is continued iteratively for the entire simulation.

The 1D solver has to be used online at each step solving a set of separate equations for each flamelet. This step along with the PDF integration increases the computational cost by a very large amount. The proposed flamelet model is based on the concept of the RIF model where we are basically trying to create a tabulated form of the RIF model. The flamelet equations are given in Equation 3.4 and Equation 3.5. These two coupled PDEs represent the unsteady flamelet equations. The boundary conditions to the above
set of equations are $Y_i(Z=0$ and $Z=1)$ i.e species mass fractions at pure oxidizer and fuel side; and $T'(Z=0$ and $Z=1)$ i.e. temperature of pure oxidizer and fuel. Given these set of boundary conditions the above PDEs can be parameterized on the basis of a set of inputs viz. $\rho$ and $\chi$. Now the solution of these PDEs will give the temporal evolution of species in the $Z$ space. The idea of the tabulation technique is to store these species mass fractions as functions of time for a range of scalar dissipation rates $\chi$. The thermochemical state is a function of $\chi$, time and $Z$. This multidimensional tabulated dataset consists of the independent variables i.e. ($\chi$, $t$ and $Z$) and the species mass fractions as the dependent variables. Consider the example of an unsteady flamelet with oxidizer boundary condition of 15 percent $O_2$ and n-dodecane as pure fuel. For a given value of the scalar dissipation rate (say 20 sec$^{-1}$) Figure 4.2 shows the temporal evolution of oxygen mass fraction in $Z$-space. The solution of the flamelet equations will give such temporal evolutions for each species as a function of $Z$. The information is stored for each species at predefined intervals of time and $\chi$.

4.2.2 Turbulence-Chemistry Interactions

It is important for the combustion model to account for the effects of turbulence-chemistry interaction (TCI) in a turbulent combustion simulation. The distribution of mixture fraction is presumed by a PDF function. In this study a beta PDF is implemented. The beta PDF function is calculated based on $\tilde{Z}$ and $\tilde{Z}^2$. The tabulation scheme is such that any presumed PDF distribution can be used. Another dimension/variable i.e. mixture fraction variance ($Z\text{var}$) is added to the earlier data set. Now the species are a function of 4 independent variables: $\chi$, $t$, $\tilde{Z}^2$ and $\tilde{Z}$. A beta PDF is constructed for each value of $\tilde{Z}^2$ and $\tilde{Z}$. This PDF is then multiplied by $Y(Z)$ and then integrated from 0 to 1. This
Figure 4.2: Temporal evolution of oxygen in flamelet space.
gives the species mass fraction for a given $\tilde{Z}^2$ and $\tilde{Z}$.

The 1D flamelet solver code along with PDF integration yields a data set with 4 independent variables and the species mass fractions as the dependent variables. This data set is a 4 dimensional data set for a given pressure. The data set can be extended for varying pressures by including another dimension of pressure to the table. In this work the model is validated against Spray A case which is a constant pressure case and hence, a 4 dimensional data set is used here.

4.2.3 Multi-Dimensional Table Generation

The flamelet code generates the temporal evolution of a flamelet from time 0 up to a time when the flamelet reaches equilibrium for a given scalar dissipation rate. The same process is repeated for different values of scalar dissipation rate. These 2 processes are independent of each other. This entire process of tabulation can be parallelized on a large scale on different processors with excellent scalability. Thus, very large tabulated data sets involving detailed chemistry mechanisms can be generated in a relatively short amount of time. The 106 species ndodecane mechanism with 420 reactions was used for chemical kinetics.

4.3 Tabulated Model Implementation in 3D Code

A tabulated data set is generated for each simulation with a given range of variables. The CFD solver calculates the mixture fraction, mixture fraction variance and enthalpy for each cell. A mass-weighted fraction of the fuel that are being injected were tracked using marker equation, which were solved for each flamelet generated given by Eq. 3.12 and Eq. 3.13. The scalar dissipation rates of each flamelet and species mass fractions are
calculated using Eq. 3.14 and 3.11. The schematic in Figure 4.3 shows the implementation in the 3D CFD code and is similar to the RIF implementation. The CFD code solves for the continuity, momentum, energy and mixture fraction equations. At every time-step iteration, $\chi_{st}$ values for a flamelet, $\tilde{Z}$, $\tilde{Z}^2$ and time $t$ are passed to the tabulated model code. A four dimensional linear interpolation scheme is used to calculate the species mass fractions from the chemistry tabulation. These species mass fractions are then used to calculate the temperature at each cell. For cases with multiple flamelets these steps are repeated for each flamelet.

4.3.1 Model Validation

The experimental data set from Spray A discussed in the previous chapters were used to test and validate the new model. The same 3D CFD model setup in RANS was implemented for the new model. The baseline Spray A case with the conditions described in previous chapter were run in a transient RANS simulation for 1.5 ms with a variable time step and the new tabulated combustion model with 20 flamelets. The temporal
Figure 4.4: Temperature and OH mass fraction predictions from tabulated model.

evolution of the flame is shown in Figure 4.4. The tabulated unsteady flamelets are able to capture the ignition delay accurately. The ignition delay from the simulation was 0.509 ms and the experimental value was reported as 0.44 ms. Unsteady flamelets are required to capture the ignition delay and the lift-off lengths. The lift-off length for the baseline case was 18.4 mm and the experimental value was 16.5 mm. Thus, the model is able to satisfactorily capture the ignition delay and lift-off lengths for the baseline Spray A condition. The lift-off length was defined as the minimum distance of the 14 percent of
max OH contour from the injector. The ignition delay was defined as the time from the start of injection to the maximum gradient point in the maximum domain temperature vs time curve. These definitions are as per the recommendations of the ECN 2 workshop. The qualitative results from the model are shown in Figure 4.4. The lift-off isocontour is shown by the black line. The upper half of the contour plot shows the temperature and lower half of the plane shows the OH mass fraction contours. OH formation is observed at 0.4 ms after start of injection without any appreciable temperature rise. The temperature rise is observed at 0.5 ms, 30mm from nozzle. This high-temperature zone then moves towards the nozzle. Quasi-steady state is reached at 1 ms.

The tabulated model was based on the structure of the RIF model. Figure 4.5 shows the qualitative difference between the RIF model and the tabulated model. The tabulated model ignites early and temperature rise can be seen at 0.5 ms. The ignition spots predicted by the two models are at the same location with both models predicting the flame propagate downstream towards the nozzle. By the time the flame reaches quasi-steady state at 1ms the flame structure predicted by both the flames are similar. Figure 4.6 shows the difference in predictions of pollutants. The C$_2$H$_2$ contour at 1.4 ms shows that the tabulated model slightly over-predicts the concentrations. The highest concentration is observed along the centre line 30 mm from the nozzle. CO predictions are also slightly over predicted by the tabualted model when compared to RIF. Higher CO concentration regions predicted by both models lie along the spray centre-line and similar in shape.

4.3.2 Temperature Sweep

The tabulated model was tested across a wide range of ambient conditions and compared with experimental data in order to prove its efficacy. The ambient temperature was
Figure 4.5: Temperature contour comparison between RIF and tabulated model.
varied from 800K to 1100K while keeping all the other parameters constant. The results are compared to those from the RIF model in the previous section. A different set of tabulated data set needs to be created for each of these simulations. The temperature of the oxidizer where \( Z=0 \) is set to the ambient temperature. This is one of the inputs to the flamelet equations and necessitates a separate table. Figure 4.8 shows the ignition delay and lift-off lengths for the different ambient temperature cases. It was observed that the tabulated combustion model is able to capture the ignition delays and lift-off lengths accurately across a wide range of temperatures. The difference between the ignition delays predicted by RIF and the tabulated model decreases with increase in temperature. Both models over predict the ignition delays when compared to the experimental data. The lift-off lengths reported by the tabulated combustion model agree well with the experimental results. Overall the new model is able to capture the trend in the ignition delay and lift-off lengths across a wide range of conditions. They are also close to the values predicted by the RIF model in the previous study.

Figure 4.6: \( C_2H_2 \) and CO mass fraction predictions from RIF and tabulated model.
Figure 4.7: Flame temperatures and lift-off lengths for 800K and 900K ambient temperatures using tabulated combustion model.
Figure 4.8: Ignition delay and lift-off lengths for Spray A across a range of ambient temperatures.
4.3.3 Injection Pressure Sweep

The effect of injection pressure on ignition delay and lift-off was studied by performing spray simulations at 50, 100 and 150 MPa at an ambient temperature of 900K. Figure 4.9 shows the ignition delay and lift-off lengths for different injection pressures compared with the experimental data and the results from the RIF model. In experiments the ignition delay decreases slightly with decreases in injection pressures, however, the lift-off length increases. The RIF model is able to capture this sensitivity in ignition delay. The tabulated model is able to capture the ignition delay close to the experimental values and under predicts the ignition delay as well as lift-off lengths. The tabulated model is also seen to capture the sensitivity for lift-off lengths across the range on injection pressures. Overall the results from the tabulated model show good agreement with the experimental results.

4.3.4 Ambient Oxygen Sweep

The tabulated model code is now validated across a range of ambient oxygen concentrations to mimic a range of exhaust gas re-circulation conditions. The Figure 4.10 compares the results with experimental data and RIF model with the same 106 specie mechanism. A new chemistry tabulation is generated a priori for each run. At low oxygen concentration of 13 percent the RIF model over-predicts the ignition delays and the tabulated model predicts ignition delays lower than the RIF model. At 15 percent oxygen concentration the over predictions for ID and LOL by both the models reduce and again the tabulated model predicts lower values compared to the RIF model. The ignition delays match closely with experiments at higher O\textsubscript{2} concentrations but the lift-off lengths are over predicted by both the models.
Figure 4.9: Ignition delay and lift-off lengths for Spray A across a range of injection pressures.
Figure 4.10: Ignition delay and lift-off lengths for Spray A across a range of oxygen concentrations.
4.3.5 Computational Cost

Turbulent combustion simulations with detailed chemistry mechanisms are computationally expensive. One of the main motivations to develop novel tabulation techniques was to reduce the computational cost. Flamelet models like RIF require sufficient number of flamelets for accurate results. A set of flamelet equations need to be solved at each time step for each flamelet. The new tabulated model aims to reduce this computational load thus enabling more detailed and complex simulations. The computational times are compared for the new model with the RIF model in Figure 4.11. All these simulations are with the 106 species mechanism. The baseline Spray A conditions are 900K ambient temperature, 150MPa injection pressure and 15 percent ambient O₂. The different cases compared here are sweeps of the baseline case with respect to each of these conditions. Each particular case is run using two different combustion models with same boundary
Table 4.1: Computational cost comparison between RIF and tabulated model for 0.25 mm minimum grid size case.

<table>
<thead>
<tr>
<th>Case</th>
<th>RIF (CPU Hrs)</th>
<th>Tabulation (CPU Hrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>800K ambient O2</td>
<td>2137</td>
<td>217</td>
</tr>
<tr>
<td>900K ambient O2</td>
<td>1234</td>
<td>222</td>
</tr>
<tr>
<td>1100K ambient O2</td>
<td>2400</td>
<td>251</td>
</tr>
<tr>
<td>100MPa injection</td>
<td>1780</td>
<td>169</td>
</tr>
<tr>
<td>50MPa injection</td>
<td>1382</td>
<td>104</td>
</tr>
<tr>
<td>13 percent oxygen</td>
<td>2372</td>
<td>224</td>
</tr>
<tr>
<td>21 percent oxygen</td>
<td>2630</td>
<td>264</td>
</tr>
</tbody>
</table>

conditions. These comparisons are for the same grid sizes and with 20 flamelets. The number of processors are also the same. The speed up was defined as the ratio of the computational time required by RIF to that of the tabulated model with same number of processors in parallel. Almost 10 times speed up were observed for most of the cases. The details of the computational cost are summarized in Table 4.1.

**4.3.6 Differences Between Tabulated Model and RIF**

Overall we observe that the tabulation code developed based on multiple flamelets is able to predict auto-ignition and flame lift-off across a wide range of temperature, injection pressures and ambient oxygen concentrations. The model is validated across a wide range of conditions proving its predictive capabilities. The tabulated model always under predicts the ignition delays and lift-off lengths compared to the RIF model. This was observed for the temperature sweep, injection pressure sweep and the ambient oxygen sweep. For these data sets the results from the tabulated model are closer to the experimental values and give an illusion that these results are more accurate as compared to RIF. However, in this model and code no extra physics have been added to solve the
chemistry in the flow field. The governing equations are the same flamelet equations for both the models. The difference is that implementing of the solution through tabulation and not solving the equations online. This infact eliminates some physics from the tabulated model. The main aim of the RIF model is to account for the temporally changing scalar dissipation rate of the flamelet through unsteady equations solved at each time step. As a result the RIF model solves the coupled flamelet PDE at every timestep with temporally changing scalar dissipation rates. This enables the RIF model to account for the ”history” of the flamelets and the solution at each time step is a strong function of the flamelet history. The tabulated models are not capable of accounting of these history effects. The tabulated models calculate the species mass fractions based on the current values of the independent variables and thus miss out on the history of flamelets. The scalar dissipation rates fro flamelets typically have a a trend as shown in Figure 3.6. The SDRs in spray flames rise to very high values when the spray starts and then decay exponentially with time. This affects the auto-ignition of the flamelet as they are very strongly dependent on SDR. The tabulated model does not take into consideration the past history of a flamelet and returns a solution based on the current state of the flamelet. Thus, it has no physics to consider this sharp drop in SDR and its effect on the current state. As a result it ignites earlier than the RIF model. This is a limitation with all tabulated models and this model as well. The study and proper quantification of these effects in a consistent framework is the motivation for the proceeding work in the next chapters. Even without the history effects the tabulated models have been able to capture turbulent flame characteristics consistently over a wide range of conditions. The difference between the predictions by the RIF and tabulated model are within acceptable range.
4.4 Conclusions

A tabulated combustion model was developed in this chapter based on the flamelet model. The combustion model is an unsteady model capable of handling large chemistry mechanisms along with turbulence-chemistry interactions. The model is a tabulation of the RIF model with multiple flamelets. The multiple flamelets help to resolve the spatial variation of scalar dissipation rates in the domain. Quantitative and qualitative results were obtained from the model for Spray A for a wide range of ambient temperatures, oxygen concentrations and injection pressures. The model was able to predict auto-ignition and lift-off lengths for diesel sprays over a wide range of conditions. Overall the results from the model closely with the experimental results and the model is validated across a range of conditions. The unsteady tabulation is implemented without using any progress variable approach. The main conclusions are summarized below:

- It is possible to implement an unsteady flamelet tabulation model without using the progress variable approach.

- A tabulated combustion model with multiple flamelets was developed and implemented. The tabulation scheme was constructed to facilitate large scale parallel processing and generate large multidimensional tables for complicated chemistry at very low costs. Any presumed PDF function can be used to account for turbulence-chemistry interactions in the current model.

- The results from the tabulated model were consistent with the predictions from the RIF model and matches closely with experimental data. The speed up achieved with the tabulation scheme was observed to be an order of magnitude for the given mesh and the problem over a range of conditions.
• The tabulated model consistently underpredicts the ignition delay and lift-off lengths compared to RIF. The physics behind these factors were discussed and the history effect of the flamelets seem to be influencing such behavior. The tabulated model does not have the mechanism to solve for flamelet histories. This provides motivation for further work and investigation of fundamental flamelet behavior and models to capture such effects.
Chapter 5

Incorporating Unsteady Effects in Flamelets

5.1 Introduction

Auto-ignition of hydrocarbon fuels at turbulent conditions is an unsteady phenomenon affected by a large number of factors spanning a wide range of length and time scales. The unsteady nature of turbulent flows coupled with unsteady chemical kinetics pose a challenge for combustion models. Mixing of oxidizer and fuel play a dominant role in auto-ignition and flame stabilization in non-premixed flames. The flamelet approach uses scalar dissipation rate (SDR) as a parameter for the mixing of oxidizer and fuel at subgrid level. Flamelets encounter temporal variations in scalar dissipation rates as they move away from the nozzle. These temporal variations could be because of the inherent unsteadiness due to turbulence or the nature of the flow. Turbulent flames in practical applications encounter such conditions and their ignition or extinction is subject to the influence of these unsteady factors.
The first part of this work develops modeling approaches that quantify the history effect and identifies variables that influence this phenomenon. A model is then developed and validated for 1D flamelets which can incorporate these history effects based on the variables of the flamelet. The modeling framework for incorporating such physics in a full 3D models with spray flames (Sandia Spray A) and multiple flamelets is presented. Comparative results from auto-ignition and flame lift-off are shown over a wide range of conditions to validate the concept and its implementation.

5.2 Evaluation of Unsteady Effects in Flamelets

1D CFDF with varying strain rates are studied numerically. The conditions from the baseline Spray A conditions were implemented on the 1D flamelet at high pressure engine conditions with EGR. The details of the 1D flamelet are presented in Table 5.1 Igniting

<table>
<thead>
<tr>
<th>Fuel</th>
<th>n-dodecane</th>
</tr>
</thead>
</table>
| Oxidizer    | $Y_{O_2} = 0.16$  
             | $Y_{CO_2} = 0.09$  
             | $Y_{H_2O} = 0.02$  
             | $Y_{O_2} = 0.71$  |
| Fuel temperature | 700K |
| Oxidizer Temperature | 900K |
| Ambient Pressure    | 59 bar  |
| Stoichiometric scalar dissipation | time varying |

flamelets encounter varying strain rates in turbulent spray flames. The auto-ignition depends on two main factors, chemical kinetics and scalar dissipation rate experienced
by the flamelet. Any fuel will have an ignition delay based on its chemistry. The ignition will also depend on the scalar dissipation rate. If the scalar dissipation rate is much higher than the quenching limit the fuel-oxidizer mixture will not ignite and vice-versa for extinction. Thus, for an unsteady ignition problem with varying scalar dissipation rate, these are the 2 main factors influencing auto-ignition in flamelets. The final auto-ignition will be the result of the coupled influence of these two factors. It has been found experimentally that the flamelet depends on the previous history of the scalar dissipation rate. i.e. the flamelet has an inertia and takes time to respond to the sudden changes in strain. These unsteady effects are referred to as the history effects. Tabulated flamelet models return solutions at every time step based on the current conditions of the flamelet. Thus, it is not possible to include history effects.

A framework needs to be developed to demonstrate the history effects on flamelets. Running an unsteady flamelet problem using tabulated libraries and comparing results to unsteady online solvers is one method to achieve this and has been done in the past by many researchers. However, in this procedure an additional interpolation error is added to the results from the tabulated models. In order to make the comparison more consistent a new methodology is proposed to suppress the history effect in flamelets without using to tabulation or interpolation.

Unsteady CFDF solver strategy is implemented in the 1D flamelet solver. This is the unsteady flamelet equation solver used by RIF solvers. In this approach the 2 PDEs are solved as per the boundary conditions for the changing scalar dissipation rates. At every time step the stoichiometric scalar dissipation rate is updated as per the strain rate profile. This implementation is same as that used in the RIF model. This model is able to account for the history effects of the flamelets along with the chemical kinetics of the problem. The auto-ignition observed will be a result of the chemistry and the dissipation
rates. Figure 5.1 describes the algorithm of the solution. The flamelet PDE are initialized to unburnt conditions. The scalar dissipation rate is updated as per the input and solved in time steps till the final time is reached.

Steady Strain assumption CFDF solver strategy: The flamelets are first initialized to unburnt conditions. The scalar dissipation rate is then updated as per the input, which is a function of time. The PDE is now solved from time $t = 0$ upto the current time step $t_1$. The flamelet solution is now available for time $t_1$. The stoichiometric scalar dissipation rate changes with time. For the second time step from $t_2$, the flamelet is again reinitialized to the unburnt condition and the PDE is solved from time $t = 0$ to $t_2$ with the new value of scalar dissipation rate. The solutions are then stored for time $t_2$. This is done iteratively for the entire simulation time. The algorithm schematic is shown in Figure 5.2. Thus,
solution at each time step is independent of the previous time step. This eliminates the history effects of the temporally changing SDR. It is important to note that this procedure eliminates only the unsteady effects of the changing scalar dissipation rate. The unsteadiness related to chemical kinetics is preserved. This procedure is computationally expensive. At every time step where solution needs to be calculated the PDEs need to be solved from time $t=0$ to that point. However, the solution of each point is independent of the previous point. As a result calculation of every time step is mutually exclusive. Thus,
the problem can be divided up into many parts and parallelized on a large scale. Message Passing Interface (MPI) routines in C were implemented to run the code in parallel and reduce computational time. The next section shows the sensitivity of these models and the effect of unsteady strain on flamelets.

5.2.1 Factors Affecting Unsteady Strain Effects

For a given flamelet problem the stoichiometric scalar dissipation rate is varied temporally. The total simulation time was set to 6.3 ms. This is the characteristic time for usual diesel engine spray injections and ignition is observed by the end of these times for baseline Spray A conditions. The 2 methods discussed in previous section are used to demonstrate the history effects in flamelets.

Consider the case where stoichiometric scalar dissipation rate changes linearly from 50 to 10 sec\(^{-1}\). The results from the unsteady solver are shown in Figure 5.3. The maximum temperature is plotted on the left hand \(y\)-axis and stoichiometric scalar dissipation rate on right. It is observed that the flamelt solution that ignores the history effect ignites early. Since the scalar dissipation rate in decreasing from a higher to a lower value, the flamelet needs some time to adjust to the new scalar dissipation rate. This has the effect of delaying the ignition. When this effect is removed the flamlet solution from the no history model i.e. the steady model ignites early as expected. These results help to quantify the effect of unsteady strain on flamelets.

Gradients in Scalar Dissipation Rates

In this part of the study history effects are evaluated for a range of gradients in scalar dissipation rates. As the magnitude of gradient in scalar dissipation rate decreases, the
difference between the flamelets with steady strain assumption and the unsteady model diminishes. For cases where the gradient is very small there is no appreciable difference in ignition delay between the 2 models. For low gradients the scalar dissipation rate changes slowly and hence the flamelets have time to adjust to the new conditions and the process is quasi steady. Hence a model that ignores history effects will suffice. However, as seen here for large gradients in SDR, the flamelets need some time to adjust to the new conditions and the solution is a strong function of the past history. A model which ignores this effect will under predict ignition delays.

5.3 Equivalent Strain Model

In order to consider these unsteady effects from a tabulated chemistry data set a model is proposed. The underlying principle behind the model is that the most recent scalar dissipation rates experienced by the flamelet contributes more to the solution of the flamelet. The equivalent strain on the flamelet is a weighted average over the history of the flamelet where the most recent history has higher weights. This claim is based
Figure 5.4: History effect on auto-ignition of flamelets under varying scalar dissipation rates for different gradients.
on the observations in the previous section. For small gradients the history effects are negligible and vice-versa. The average of most recent histories for a flamelet experiencing small gradients will be closer to the current value of scalar dissipation rate. Hence small differences are observed between the unsteady and the no history model for lower gradients. For higher gradients in SDR, the average over most recent histories will lead to an equivalent SDR with a large difference with the current SDR at a given time step. As a result we see large difference between the unsteady and steady strain models. This hypothesis is further put to test through 1D flamelet and 3D spray flame validations.

### 5.3.1 Weight Function

A step function [54] is constructed to carry out the weighted averaging of the flamelet history. This weight function is given by equation 5.1.

\[
w(t) = \frac{ae^{cr} + be^{rt}}{e^{cr} + e^{rt}}
\]

(5.1)
where \( a = 0, \ b = 1 \) and \( r = 20 \) This is a step function and the parameters \( a \) and \( b \) control the lower and upper limits. The parameter \( r \) controls the slope of the step and \( c \) controls the position of the step from the origin. These parameters except \( c \) are fixed and have not been changed in the entire study. Figure 5.5 shows the plot of weight function. The range of the weight function is 0 to 1. An equivalent strain is calculated using weight averaging for a flamelet with varying SDR. The temporal variation of SDR is plotted against non dimensional time. The parameter \( c \) controls the position of the step from 0. The slope \( r \) is set to 20 in this work. At each time step of the flamelet calculation, the history of the scalar dissipation rate is known. The equivalent strain is calculated using the following equation:

\[
\chi_c = \frac{\sum_0^t \chi(t)w(t)}{\sum_0^t w(t)}
\]  

(5.2)

In the weight function \( t = 0 \) represents time=0 and \( t = 1 \) represents the current time-step. Consider the parameter \( c \) to be 0.7. When the equivalent SDR is calculated using Equation 5.2, the SDRs after 0.7 will contribute more towards the average and the SDRs before 0.7 will gradually contribute less to the average. Thus, the most recent history will contribute more to the equivalent strain. Moreover this process can be controlled by the variation of \( c \). Smaller values of \( c \) will shift the step function to the left and result in more time averaging and vice-versa. This equivalent strain is then used in the ”no history” 1D model to mimic the implementation of this equation in a tabulated model. The following section shows the effect of this model and the influence of the correction factor \( c \).
5.3.2 Model Validation in 1D Code

The 1D CFDF flamelet problem is solved with varying gradients in SDR. The proposed model is applied to the 1D solver which neglects history. The parameter $c$ controls the amount of time averaging over the history of the flamelet. Smaller values of $c$ will lead to more averaging. An equivalent strain is calculated at each time step by the weighted averaging process where the most recent history is given more weight. The results from parametric variations in $c$ are shown in Figure 5.6. It is observed that the use of the equivalent SDR shifts the maximum temperature curve towards the unsteady results. For smaller gradients higher values of $c$ are enough to predict the unsteady and vice-versa i.e. more time averaging is required for higher gradients. In all these cases the final SDR was $10 \ sec^{-1}$. For every gradient there exists an optimum value of $c$ that will predict the auto-ignition as per the unsteady results. Thus, we can predict the unsteady results using a tabulated data set calculated without history effects.

Some more tests reveal that the optimum value of $c$ is also dependent on the final scalar dissipation rate. The 1D flamelet cases with the new model were run for the same gradients but for different values of scalar dissipation rates and the results are presented in Figure 5.7. These results show that the optimum value of $c$ that can predict auto-ignition close to unsteady results are also a function of the final scalar dissipation rate. In the first case the scalar dissipation rate changes from 25 to 10 and in the second case changes from 35 to 20. For the first case, $c=0.4$ provides a good approximation, however, for the second case, $c=0.3$ is a slightly better approximation. The correction factor $c$ which controls the weighted averaging is a function of the stoichiometric scalar dissipation rate gradient as well as the absolute value of the scalar dissipation rate. In order to implement a predictive CFD model without parameter tuning a scheme was developed that calculates
Figure 5.6: History effect on auto-ignition of flamelets under varying scalar dissipation rates for different gradients.
Figure 5.7: Auto-ignition of flamelets for different scalar dissipation rate gradients and magnitudes.

this correction factor $c$ based on $\frac{d\chi_{st}}{dt}$ and $\chi_{st}$. i.e. $c = f(\chi_{st}, \frac{d\chi_{st}}{dt})$ In order to achieve this a number of cases are run iteratively for different values of $c$ for a given value of $\frac{\partial \chi_{st}}{\partial t}$ and $\chi_{st}$. The value of $c$ which predicts the auto-ignition closest to the unsteady results are selected and tabulated in a 2D table. The 2D table represents the correction factor as a function of $\frac{d\chi_{st}}{dt}$ and $\chi_{st}$. This 2D table is shown in Table 5.2.

5.3.3 Implementation in the 3D Code

A model capable of including history effects was developed for 1D flamelets. The secondary table is a 2 dimensional table where the correction factor $c$ is stored as a function of $\chi_{st}$ and $\frac{d\chi_{st}}{dt}$. The tabulation scheme’s coupling with the 3D CFD solver is dis-
Table 5.2: Secondary tabulation showing values of $c$ as functions of $\frac{d\chi_{st}}{dt}$ and $\chi_{st}$.

<table>
<thead>
<tr>
<th>$\chi_{st}$</th>
<th>$d\chi_{st}/dt$</th>
<th>$1.1 \times 10^5$</th>
<th>$0.95 \times 10^5$</th>
<th>$0.79 \times 10^5$</th>
<th>$0.63 \times 10^5$</th>
<th>$0.47 \times 10^5$</th>
<th>$0.31 \times 10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.21</td>
<td>0.23</td>
<td>0.289</td>
<td>0.321</td>
<td>0.403</td>
<td>0.380</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.654</td>
<td>0.212</td>
<td>0.261</td>
<td>0.292</td>
<td>0.329</td>
<td>0.385</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.639</td>
<td>0.576</td>
<td>0.248</td>
<td>0.217</td>
<td>0.319</td>
<td>0.400</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>0.209</td>
<td>0.216</td>
<td>0.453</td>
<td>0.267</td>
<td>0.217</td>
<td>0.327</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.289</td>
<td>0.290</td>
<td>0.209</td>
<td>0.189</td>
<td>0.380</td>
<td>0.209</td>
<td></td>
</tr>
<tr>
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<td>0.392</td>
<td>0.302</td>
<td>0.289</td>
<td>0.188</td>
<td>0.190</td>
<td></td>
</tr>
</tbody>
</table>

cussed in the schematic. For simulations with multiple flamelets, each flamelet has its own stoichiometric scalar dissipation rate. At any given time-step the tabulated combustion model calculates the species based on the mixture fraction, mixture fraction variance, scalar dissipation rate and time. In this case the correction factor $c$ is interpolated from the secondary 2D table. Using this value of $c$ and equation 5.2 an equivalent stoichiometric scalar dissipation rate is calculated from the temporal history of $\chi_{st}$. This equivalent $\chi$, is used to retrieve the species from the multidimensional chemistry tabulation. At every time step for every flamelet the value of $c$ is calculated based on $\chi_{st}$ and $d\chi_{st}/dt$. This implementation is shown in the schematic in Figure 5.8 for a single flamelet. For multiple flamelets the implementation is the same and the procedure is repeated for each flamelet in an iterative manner. The CFD model set-up is same as the baseline setup used for the tabulated model in Chapter 4 with 20 flamelets and the 106 species 420 reactions mechanism.
5.3.4 Validation of Equivalent Strain model in the 3D Code

The use of an equivalent $\chi_{st}$ based on a weighted averaging process was implemented in 1D flamelets. Investigations showed that implementation of this model in 1D flamelets could predict auto-ignition results close to unsteady models. This concept of accounting for history effects from steady libraries is tested for a 3D spray flame simulation in a RANS framework. The Sandia Spray A was modelled using the CFD set-up discussed in Chapter 2 along with the tabulated combustion model implementation in Chapter 4. It was observed that the tabulated model was unable to capture history effects and hence, under predicted the ignition delays and lift-off lengths compared to the RIF model. The baseline case with 900K ambient temperature was evaluated with the new model. The results are compared to the tabulated model and the RIF model. Figure 5.9 shows
the maximum temperature as a function of time predicted by the three models. The tabulated model ignites before the RIF model as its not affected by the history effects. The equivalent strain model closely follows the auto-ignition pattern of the RIF model. The ignition delay closely matches that of the RIF model. This result validates the equivalent strain model. Similar results were observed with lift-off lengths reported in Figure 5.10. The lift-off length predictions are significantly closer to those predicted by the RIF model.

Figure 5.12 shows the qualitative results demonstrating history effects in Spray A. The OH contours are plotted at different time-steps with the adaptive mesh refinement visualization. The upper half shows the results from the tabulated model and the lower half of the spray axis shows results from the equivalent strain model implementation. The tabulated model starts igniting at 0.5 ms whereas the tabulated model with history effects i.e. equivalent strain model ignites later. The flame structure predictions are similar reaching a quasi steady state by the end of 1 ms.
Figure 5.10: Lift-off lengths predicted by RIF model, tabulated model and tabulated model with history effects.

The new tabulated model with history effects is validated across a range of injection pressures from 50 MPa to 150 MPa. The results are compared against the RIF model and the tabulated model in Figure 5.13. It was observed in previous sections that the tabulated combustion model under predicts the ignition delay for the given range of injection pressures when compared with the RIF model. The new model predicts longer ignition delays ignition delays closer to the RIF predictions. The same trend is observed for the lift-off lengths. Overall, we observe that the new model is able to capture the unsteady effects resulting in an increase in ignition delay and lift-off lengths across the injection pressures.
5.4 Conclusions

The first part of the chapter developed a comparative methodology and demonstrated the impact of flamelet histories over steady strain assumptions for flamelets with unsteady scalar dissipation rates at engine relevant conditions. It was further demonstrated that the history effects are directly proportional to the temporal gradients in $\chi_{st}$ experienced by the flamelet. A concept to account for unsteady effects in tabulated combustion models was proposed. The concept is to calculate a weighted average of the stoichiometric scalar dissipation rate over the flamelet history. The weighted averaging uses higher weights for the most recent histories. The model is validated in 1D CFDF problems and full 3D spray flame simulations. Auto-ignition and lift-off length results over a wide range of ambient temperature and injection pressure conditions validate the model. Quantitative and qualitative results from Spray A were presented. The main conclusion from this part of the study are as follows.

- The magnitude of temporal gradient in stoichiometric scalar dissipation rate of a flamelet determines the history effect. The difference in auto-ignition due to history effects is directly proportional to the magnitude of $\partial \chi_{st}/\partial t$. For flamelets experiencing very small gradients in scalar dissipation rates the history effects are negligible. When $\chi_{st}$ changes rapidly over a short period of time, the flamelet takes some time to adjust to the new conditions and this has a strong influence on auto-ignition. Thus, steady $\chi$ assumptions cannot predict auto-ignition correctly. Tabulated flamelet models are not capable of accounting for these effects.

- An equivalent $\chi_{st}$ can be calculated based on the history of the flamelet using a weighted averaging averaging procedure. When this equivalent $\chi_{st}$ is used along with steady strain assumptions the model seems to capture the effect of the history
of the flamelet. This was demonstrated in 1D flamelets. Further a scheme was constructed to apply this model for 3D spray flames.

- The new model was implemented in a 3D RANS code. Comparative studies show that tabulated combustion models can account for history effects in 3D spray combustion simulations. The results across a range of temperature and injection pressures show consistent improvement over predictions from tabulated models with steady scalar dissipation rate assumptions.
Figure 5.11: Ignition delay and lift-off lengths predicted by RIF model, tabulated model and tabulated model with history effects across ambient temperatures.
Figure 5.12: History effect on ignition of Spray A: OH contours from tabulated model and tabulated model with history effects.
Figure 5.13: Ignition delay and lift-off lengths predicted by RIF model, tabulated model and tabulated model with history effects across injection pressures.
Chapter 6

Conclusions

Modeling approaches for reacting diesel sprays were implemented in a 3D RANS code with adaptive meshes. Grid convergent simulations with detailed chemistry mechanisms were implemented for constant vessel combustion experiments as well as single cylinder diesel engines. Two different chemistry mechanisms were implemented with different combustion models. Results from the multi-flamelet RIF model in Chapter 3 demonstrate the validation of RIF code across a wide range of diesel injection conditions. The RIF model was able to predict auto-ignition and lift-off across a range of conditions. Moreover, a systematic approach was developed for determining the minimum number of flamelets required for convergent results. This was further validated in engine cases. Comparative study between the finite-rate chemistry model and the RIF model showed the differences in the two models.

A tabulation technique was proposed based on the multi-flamelet RIF model. The tabulation structure was such that it could facilitate large scale parallel processing for complicate chemistry mechanisms. Multidimensional chemistry tables were generated for the 106 species n-dodecane mechanism. The new tabulated model was validated across
a wide range of Spray A conditions. The auto-ignition and flame lift-off results matched closely with the experimental values for a range of ambient temperatures, oxygen concentrations and injection pressures. The quantitative difference between the RIF model and the tabulated model were discussed. The tabulated model was observed to be 10 times faster than the RIF model for the same number of flamelets and mesh across a wide range of cases. This shows the efficacy of tabulated models. The tabulation of the RIF model has the effect that it fails to capture the unsteady strain effects i.e. the history effect of the flamelet. Hence the tabulated flamelet model under-predicts ignition delay and lift-off consistently as compared to RIF across a wide range of conditions. These effects were demonstrated with the help of 1D counter flow diffusion flamelet experiments in the next section.

Two different modeling approaches were constructed for a comparative study between the steady strain assumption and unsteady strain assumption in flamelets. The steady strain assumption mimics the solution from a tabulated model i.e. neglects the history effect on the flamelet. The unsteady model is the traditional 1D unsteady flamelet equation solver which time advances the PDEs thus taking into account the history effects. These two models were subject to unsteady strain rates over a range of gradients. Comparative studies show that the history effect is more pronounced for cases where the magnitude of temporal gradient in scalar dissipation rate is high. An equivalent strain model was proposed that calculates an equivalent strain based on the history of the flamelet and the gradient of scalar dissipation rate. Application of this model to 1D flamelets with steady strain assumption showed that auto-ignition results matched the results from the unsteady solver. This implied that history effects can be considered even in tabulated models. This model was further implemented in the 3D code. The auto-ignition and lift-off results closely match the predictions from the RFI model. This indicates that the new
concept can enable tabulated combustion models to capture unsteady strain effects.

6.1 Future Work

The RIF model with multiple flamelets are required to model the unsteady strain effects in flamelets. However, owing to the high computational costs these type of models are not used for practical applications. Moreover, combustion CFD simulations need to deal with large chemistry mechanisms and large meshes in order to be predictive in nature. The turbulent mixing of fuel and oxidizer coupled with the unsteady nature of chemical kinetics pose a challenge for combustion models. As a result a number of assumptions and reduced order modeling approaches have been adapted by the industry. The development of tabulated combustion models has enabled the use of detailed chemistry at lower computational costs. The tabulated combustion modeling techniques developed in this work has some major implications for turbulent combustion modeling for non-premixed flames.

The tabulated model is significantly faster compared to the RIF model. Moreover the equivalent strain model coupled with the tabulated model can enable the model to capture history effects. This means that high fidelity combustion simulations are achievable at comparatively lower computational costs. With such approaches either the cost is reduced to a large extent or a much larger problem can be solved with the same amount of computational resources. One example would be the implementation of detailed chemistry mechanisms with thousands of species and reactions. The current state of the art for engine simulations is to reduce detailed mechanisms to a range of operating conditions. Moreover such reduction is accompanied by errors in ignition delays. Using thousands of species in engine simulations is costly and would need very large memory and com-
putational power. The implementation of high fidelity tabulated models can be used to solve problems with such chemistry. Moreover the tabulation process can be parallelized on thousands of processors and tabulated once. These tabulations can then be used successively by the CFD simulations and run for complex problems with large meshes on relatively smaller computing clusters. The combustion models developed in this study can be used with LES. LES simulations need very small grid sizes. The tabulation approach coupled with detailed chemistry has the potential to reduce the computational costs of highly complex simulations and give new insights in engine combustion.
REFERENCES


