Large Eddy Simulation of Turbulent Premixed Combustion in Gas Turbines

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LARGE EDDY SIMULATION OF TURBULENT PREMIXED COMBUSTION IN GAS TURBINES

A Dissertation

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Dedicated to my family and all of my friends...those who have come and gone, those who have been there, and those whom I've yet to meet
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Abstract

An artificially Thickened Flame (TF) approach based on LES framework is used to model the turbulent premixed combustion in gas turbine combustors. A number of variants of the Thickened Flame approach including a modified version of TF model have been studied in details. In the TF model, the flame front is artificially thickened to resolve on LES computational grid. With this approach, reaction rate modeling does not require any ad-hoc closure assumptions. However, suitable modifications have to be made to compensate for flame thickening. To verify the predictive capability of the models, a stoichiometric methane-air flame on Bunsen burner type geometry has been simulated and the TF model predictions compared with experimental data as well as with other model predictions.

As a part of this research, turbulent flow over a backward facing step, isothermal swirling flow in a confined geometry have also been studied and predictions are compared with experiments. Good agreement with data is obtained that validates the LES model used.

The validated LES based TF model is used to investigate flashback behavior in hydrogen enriched premixed flame in a swirled combustor. Firstly, non-reacting and reacting flows with natural gas are studied, followed by hydrogen enriched combustion. In general, the LES predictions for both reacting and non-reacting cases are found to be in good agreement with measurements. In non-reacting flow conditions, the recirculation zones (WRZ, CRZ and CTRZ) are clearly observed, especially at high Reynolds number. Moreover, the observations reveal that higher combustibility of hydrogen causes Combustion Induced Vortex Breakdown driven flashback due to complex interaction of chemical reaction in swirled burner, resulting in faster flame propagation into the upstream mixing tube. In particular, combined effect of baroclinic production and vortex stretching accelerates the upstream flame propagation in hydrogen-enriched
mixture, while only methane shows stable behavior. Further, the effect of swirl strength, premixedness and geometry has also been studied on flashback behavior of hydrogen enriched mixture. Flame flashback is always observed at higher swirl strength irrespective of level of premixedness and burner geometry, whereas the premixed systems exhibit stable behavior while operating under lower swirl strength.
Chapter 1 Introduction

1.1 Gas Turbine Combustion

Combustion is represented by a chemical reaction and is accompanied by the production of heat and light. However, the classical definition according to Webster’s dictionary is “rapid oxidation generating heat, or both light and heat; also, slow oxidation accompanied by relatively little heat and no light” (Turns, 2000). Combustion has a huge impact in our daily lives starting from household uses like cooking and heating to industrial applications like automotive industries, manufacturing sectors and power generation plants. The majority of new power generation in the last decade has come from land-based gas turbines. The reasons for this are: higher efficiencies, ability to generate power in smaller increments compared to traditional power plants, compact construction, low NOx emissions as well as the capability of using different blend of fuels. To this end, the gas turbine combustion has become a particularly promising approach for clean energy generation.

In gas turbine combustion, hydrocarbons are the fuel source which essentially contain hydrogen and carbon atoms. Theoretically, with complete combustion, oxygen in air must combine with all the carbon and hydrogen atoms in the fuels to produce carbon dioxide and water respectively, leaving the nitrogen in the air unaffected. However, in reality, the combustion processes can produce unburned hydrocarbons (UHC) and unwanted, harmful pollutants (e.g. NO) as by-products.

The major concern associated with gas turbine combustion is environmental pollution, and pollutants such as NO potentially have health hazards. The exhaust of a gas turbine consists of particulate matter, such as soot, fly ash, various aerosols etc. (Glassman, 1996; Turns, 2000), and gases including carbon dioxide (CO2), carbon monoxide (CO), water vapor (H2O), sulfur oxides
(SO₂ and SO₃), nitrogen oxides (NOₓ), unburned hydrocarbons (UHC) and excess atmospheric oxygen and nitrogen. Carbon dioxide (CO₂) and water vapor (H₂O) are the natural consequences of complete combustion of hydrocarbon fuel. However, CO₂ contributes to the global warming and can only be reduced by burning less fuel. Sulfur oxides are toxic and corrosive. They often form sulfuric acid in atmosphere. Since all the sulfur in fuel is oxidized to SO₂, the only way it can be avoided is by removing sulfur before combustion. Carbon monoxide is toxic and reduces the oxygen absorption capacity of blood, although in high concentrations, can cause asphyxiation and even death. Unburned hydrocarbons are not only toxic, but they also combine with nitrogen oxides to form photochemical smog. Particulate matter is not generally considered as toxic but has a strong association with asthma and other respiratory diseases and atmospheric pollution. Nitrogen oxides (NOₓ) mostly contribute to ground level smog, damage to plant life and acid rain. NOₓ emissions at higher altitudes contribute to the depletion of the stratospheric ozone layer through the following reaction mechanism (Turns, 2000)

\[ NO + O_3 \rightarrow NO_2 + O_2 \]  \hspace{1cm} (1.1)

\[ NO_2 + O \rightarrow NO + O_2 \]  \hspace{1cm} (1.2)

Unfortunately, supersonic aircraft are required to operate at such altitude. Ozone depletion results in a substantial increase in ground level ultraviolet radiation which, in turn, increases the possible occurrences of skin cancer.

1.2 Low Emission Combustors: Design and Development

Increasing restriction on pollutant emissions, particularly nitrogen oxides, is the key driver in the development of modern day gas turbine combustors. Traditional combustors that were used before environmental issues became important operated on non-premixed mode and hence led to unacceptably high levels of thermal NOₓ. Stringent emission requirements over the
last decade has required a complete re-design of the air-fuel delivery system with a focus on low-emission designs. Factors that mainly control the emissions from combustors are considered to be (Lefebvre, 1995):

1. The primary zone temperature and equivalence ratio.
2. The degree of homogeneity of the primary zone combustion process.
3. Residence time in primary zone.
4. Linear-wall quenching characteristics.

In practice, there are three major processes (Leckner, 2002) that are undertaken to control emissions.

- **Post-treatment of Exhaust Gases**

  In this method, the exhaust gases are allowed to pass through a fixed catalytic bed. Selective catalytic reduction (SCR) is one of these processes which uses ammonia to convert the exhaust NO\textsubscript{x} into molecular nitrogen and water vapor. Exhaust gasses are primarily passed through an oxidation catalyst and then mixed with ammonia. The oxidation catalyst takes CO and UHC from the exhaust gas, and then other base metal catalysts in presence of ammonia react with NO\textsubscript{x} to form N\textsubscript{2} and H\textsubscript{2}O through the following reaction mechanism (Lefebvre, 1995)

\[
4NH_3 + 6NO \rightarrow 5N_2 + 6H_2O
\]  

(1.3)

\[
8NH_3 + 6NO_2 \rightarrow 7N_2 + 12H_2O
\]  

(1.4)

Using this method, almost 90% NO\textsubscript{x} can be removed from exhaust gasses. However, there are few problems associated with SCR units, such as the feed back control systems for ammonia need to be robust, monitoring systems for feed back control need to be continuous, and the equipment is generally large in size and weight. Despite these drawbacks, this method is quite widely used.
except in aircraft engines where this approach is not feasible.

- **Fuel Preparation**

  Preparation of fuel has enormous impact on emissions. In recent times, the trend is to use natural gas as the fuel of choice. The main component of natural gas is methane (CH₄) which has a lower stoichiometric flame temperature compared to the higher hydrocarbons and therefore reduce the formation of thermal NOₓ. Additionally, burning CH₄ can release an equal amount of heat with less CO₂ emission compared to other heavier hydrocarbon fuels due to its higher heating value and lower molecular weight (Turns, 2000; Glassman, 1996). With the recent emphasis on coal gasification, the most recent trend is to use H₂ under lean and premixed conditions, close to the lean blow out limit.

- **Control of Combustion Chamber Conditions**

  At this stage, it has been a difficult situation for the combustion community to meet the emission requirement without losing the combustion efficiency. The approaches adopted to improve the combustion efficiency (higher temperature, lower residence times) potentially conflict with the goal of decreasing the pollutant emissions (Turns, 2000; Lefebvre, 1995; Bahr, 1999).

  The NO formation mechanisms can be broadly categorized into three different chemical routes: (1) the extended Zeldovich (or thermal) mechanism, (2) rapid formation, and (3) fuel-nitrogen mechanism (Turns, 2000; Glassman, 1996). In the Zeldovich mechanism the NO formation is strongly dependent on the flame temperature, and the formation rate varies exponentially with the flame temperature. This mechanism becomes unimportant below the temperature level of 1850K (Lefebvre, 1995). The rate of NO formation is slower than the fuel oxidation rate, however, in the postflame region this rate is almost linear with time but does not attain its equilibrium state (Lefebvre, 1995). Based on these facts, it is obvious that NO emissions are decreased by reducing the flame temperature and residence time. On the contrary, CO production becomes significant
at very low flame temperature, due to the fact that oxidation rate is low at low temperature as indicated in Figure 1.1 (Lefebvre, 1995).

![Graph showing influence of primary zone temperature on CO and NOx](image)

**Figure 1.1: Influence of primary zone temperature on CO and NOx (Lefebvre, 1995)**

It is seen from Figure 1.1 that the low levels of CO and NO$_x$ are obtained within a narrow band of combustion temperature; for example, when temperature is between 1680 and 1900 K, the CO and NO$_x$ levels are below 25 and 15 ppm, respectively. Hence the underlying concept for developing a low-emission and efficient combustor is that the combustion temperature should be maintained within a fairly narrow band.

Combustion processes are generally classified as premixed, non-premixed (or diffusion) and partially premixed, depending on the state of mixedness of the reactants. In a non-premixed flame, the fuel and the oxidizer are separately injected into the combustion chamber, and the burning as well as mixing takes place at the same time across the fuel and oxidizer interface. However, premixed combustion requires the fuel and the oxidizer to be mixed completely at the molecular level before the reaction is allowed to take place. In partially premixed combustion, the fuel and oxidizer are injected separately, but mixed partially by turbulence and then the combustion takes
place in a stratified medium once the mixture is ignited. The spark-ignition engine is an example of premixed mode of combustion, while the candle burning is an example for non-premixed combustion. Practical devices like gas turbines have been designed and operated over a range of premixed conditions. Aero-engines operate in a fully non-premixed mode, while land-based gas turbines operate primarily under premixed conditions.

In turbulent non-premixed combustion, the fuel and oxidizer are injected separately into the combustion chamber where they mix and burn. The mixing occurs initially on macro scale by turbulent convection, and is then further mixed at small scale by molecular diffusion across a wrinkled interface. Non-premixed burner are less prone to combustion instabilities, flame flashback, blow-out, and acoustical and mechanical vibrations. In non-premixed combustion the local peak flame temperature always remains close to the adiabatic temperature due to characteristics of the reaction which always takes place around the stoichiometric surface. Unfortunately, due to the higher flame temperature thermal NO\textsubscript{x} production generally becomes significant. As a result, the non-premixed combustion is not preferred in the development of low emission combustors (Turns, 2000) (Lefebvre, 1995).

In premixed combustions, the fuel and oxidizer is completely mixed before entering the combustion chamber. The flame temperature can be maintained below the adiabatic temperature by controlling the equivalence ratio; for low equivalence ratios or lean conditions the flame temperature is low enough, so that NO formation is minimized. This philosophy is therefore preferred in the development of low NO\textsubscript{x} emission combustors. However, premixed combustion suffers from the problem of combustion instabilities driven by thermo-acoustic coupling.

Another major problem in premixed combustion is flame flashback. Flashback means the flame starts propagating upstream of the dump plane and enters the mixture passage without quenching (Turns, 2000). It may result in an explosion or cause severe damage to the injector as well as
the incoming delivery-system pipe walls. When the local flow velocity becomes lower than the local flame speed, flashback phenomena occur. This generally occurs in the fuels with high flame speeds or when the fuel air delivery system has regions of low velocity. Further, since premixed combustion is generally operated close to the lean blow out limit, occasional extinction of the flame is encountered.

Specific configuration designs (Lefebvre, 1995) are discussed below.

- **Variable Geometry Combustor**

  In this combustor, large quantities of air are admitted at the upstream and maintain the combustion temperature within an ideal range as well as to provide adequate cooling air for maximum power conditions. Due to the low combustion temperature, this kind of combustor potentially reduces the main pollutants without hurting the combustor’s performance. However, this kind of design suffers from many drawbacks, such as complex control and feedback mechanisms (which eventually tend to increase cost, weight and reduce reliability) and operational reliability.

- **Rich-burn, Quick-quench, Lean-burn Staged Combustor (RQL)**

  This design operates on the concept of staged burning. The combustion is initiated in a fuel-rich state at equivalence ratio between 1.2 and 1.6. Thus reduces NO$_x$ formation by lowering both the available oxygen and flame temperature. Higher equivalence ratio are generally desirable from NO$_x$ standpoint, but it leads to excessive soot formation and smoke. The flow out combustion products, which are coming out from the initial zone, rapidly mix with the cold air in the quench mixer (the equivalence ratio reaches between 0.5 and 0.7), and reduce their temperature to a level at which NO$_x$ formation is negligibly small. Finally, the lean mixtures burn out in the lean-burn staged zone. The key part for design consideration of a efficient RQL, is the quick quench mixer. The other inherent problem of RQL is that the NOx production becomes much more
significant if the transition from the rich zone to lean zone does not take place rapidly resulting in near-stoichiometric mixtures group to exist for longer times, which increases NO\textsubscript{x} and decreases the effectiveness of the RQL combustor.

- **Staged Combustor**

  The basic concept of this type of combustor is that the whole combustor chamber is divided into several staged or arranged with several zones or sub-chambers. The philosophy behind this type of setting is that only one zone works at low power settings, while as the power increases, more and more zones come into effect. This kind of staging becomes useful to operate the combustor over the whole power range while keeping the combustion temperatures within the expected low-emissions window. The staged combustor is usually categorized as radial staging or axial staging based on the arrangement of the zones.

- **Lean Premixed Combustor**

  This is a type of dry low NO\textsubscript{x} combustor where the operational concept is to eliminate the local high temperatures by mixing fuel and air upstream of the combustion zone. Based on the type of fuels used, they are referred to as Lean Premixed/Prevaporized (LPP) combustors (using liquid fuels) or Lean Premixed (LP) combustors (using gaseous fuels). The underlying principle is to supply the primary combustion zone with a completely homogeneous mixture of fuel and air keeping the equivalence ratio very close to the lean blow-off limit. As the equivalence ratio is maintained closer to the lean blow-off ratio, it reduces the output of NO\textsubscript{x}, but exhibits instabilities inside the combustion chamber, and hence the combustion becomes more unstable. However, one major advantage of LPP/LP combustion is that the soot formation is significantly low, the heat release is reduced and consumes less amount of cooling air. Typically, the temperature in LPP/LP combustors is somewhere around 1900 K, which is not only good for lower NO\textsubscript{x} formation, but also good for obtaining low CO and UHC as the residence time increases. Besides the advantages,
the major drawbacks of LPP/LP system are acoustic’s resonance, occurrence of autoignition or flashback as longer time is required to achieve complete evaporation and mixing, potentially resulting in severe damage to the combustor.

- **Catalytic Combustor**

  Catalytic combustion is known as ‘flameless’ process, which allows the combustion to take place at temperature well below the normal flammability limit. Generally, in catalytic systems which requires very uniform mixtures at the catalyst inlet, the fuel and combustion airflow are mixed upstream of the reactor to provide lean and homogeneous mixtures at the catalytic-combustor inlet. Typically platinum or palladium are used as catalyst materials to enhance fuel oxidation that occurs on the reactor substrate surfaces. This reactor produces really low levels of NOx, CO and UHC as well. Additionally, the most common stability problem with lean combustion burners can be eliminated in this type of combustor and operated under steady combustion with no dynamic pressure instabilities even with very lean mixtures. The limited life time of catalysts and incomplete fuel oxidation have been a major problem with this type of combustor.

  There are few dry low NOx (DLN) or dry low emission (DLE) combustors that have been developed successfully and available in the market; one is the General Electric (GE) LM6000 engine and another is the Asea Brown Boveri (ABB) combustor. They are briefly described below.

  Figure 1.2(a) shows a schematic of GE’s LM6000 DLE combustor (Bahr, 1999; Gabrielsson & Hermann, 2002) which consists of 75 premixer modules in its combustor dome. The distribution of these premixer modules is such that outer and middle rings have 30 premixers while the inner one has 15. The air is allowed to flow through three annular rings of premixers into the combustion chamber. To achieve low emissions, the design of premixer modules becomes very important. Each premixer is manufactured with different components that includes counter-rotating inner and
outer swirler assembly and fuel supply manifold. Figure 1.2(b) shows the drawing of one of the premixers.

Figure 1.3 shows the dual fuel EV burner (Strand, 2002), which is a conical premixed combustor module and developed by ABB company. Two offset half cones, which create two axial air inlet slots, is a unique feature of this type of burner. The flame stabilization usually occurs in the free space near the burner outlet due to the sudden breakdown of the swirling flow. The fuel/air mixing takes place rapidly in swirling flow as soon as the gaseous fuel is injected into the airstream inside the half cones. In case of liquid fuels, an atomizer is used to inject fuel at the
apex of the premix cone that allows the fuel to evaporate and mixed with the air. The combustion temperature can be controlled by injecting water or steam into the cone, if required. As the flame stabilizes due to vortex breakdown, no diffusion, pilot stage or mechanical flame holder is needed to improve the stability of the premixed flame.

1.3 Combustion Diagnostics and Tools

To better understand combustion processes, there are plenty of sophisticated measuring equipment and many advanced experimental methods are available. Some of them are as follows:

- Laser Doppler Velocimetry (LDV) for velocity measurement.
- Stereoscopic Particle Image Velocimetry (SPIV) for velocity measurement.
- Intensified CCD imaging of flame chemiluminescence.
- Planar Laser-Induced Fluorescence (PLIF) for concentration of radicals and some species, such as CH, OH.
- Schlieren technique detects gradients in the refractive index (or density) for visualization of flame fronts.
- Raman-Rayleigh scattering technique for mixture fraction, temperature and the concentration
of major species.

- Coherent Anti-Stokes Raman Scattering (CARS) for temperature measurement.

Over the last few decades, extensive experimental studies have been conducted to properly understand the combustion phenomena using the above-mentioned techniques and measuring equipment. These studies have been really valuable in successfully capturing turbulence and flame structures, interaction between turbulence and combustion, and hence have become standard tools in combustion research. Kaminski et al. (2000a; 2000b) captured the evolution of turbulence in real time using high-speed PLIF technique, and did an qualitative comparison with 2-D DNS and 3-D LES results. Nygren et al. (2002) used three-dimensional PLIF techniques to study the combustion problems. In recent times, joint measurements applying two or more of these techniques altogether, have become really promising. Hult et al. (2000) used a time resolved PLIF and instantaneous PIV measurements techniques to capture the dynamics of turbulent/chemistry interaction in real time. Chen et al. (1997) conducted an experiment for a high-speed hydrocarbon flames using Rayleigh scattering and laser-induced fluorescence simultaneously. Chen et al. (1996) used jointly LDA and LIPF techniques to study the detailed flame structure of highly stretched turbulent premixed methane-air flames. Kohse-Höinghasus et al. (2004) published a review article on combustion diagnostic techniques based on laser equipment recently. Fureby et al. (2007) did some experiments on a multi-swirl gas turbine combustor using LDV and PIV techniques. Depending on the data obtained from these measuring techniques, the understanding of the complex physical and chemical mechanisms that govern turbulent combustion has become better and better gradually.

The experimental studies, however, do have plenty of limitations. Design, manufacture, preparing the experimental setup take lot of time, even then these expensive setup and measuring equipment, especially, can not provide detailed information of the complete flowfield. Having
these limitations, the experimental studies are not that much useful in combustor design directly, however, provide lot of information to have better physical understanding of the combustion process as well as databases for validation or development of the combustion prediction models.

Computational fluid dynamics (CFD), on the other hand, has become a really promising tool to simulate or predict the fluid flow by solving a set of partial differential equations. However, the fact of matter is recent progress in computer technology and improvement of numerical methods, has helped CFD to reach a highly esteemed level in studying flow problems and developing flow related equipment for complex geometries, such as airplanes, motor vehicles, gas turbines, and so on. Having proper models and enough computing resources, CFD simulations can provide detailed information of the flow field for a particular problem in a cost effective manner compared to the corresponding experiments. CFD has been successfully applied to solve many industrial problems in last few decades. Moreover, recently, there are many powerful commercial CFD packages are available in the market, such as Fluent, CFX, and StarCD.

1.4 Motivation and Objectives

Land-based gas turbine combustors are operated on premixed mode and encounter plenty of problems associated with flame flashback, blow-off, thermo-acoustic instabilities and emissions. Most of the earlier studies including experimental and numerical techniques provide useful information; however, a thorough understanding of the underlying phenomena that lead to efficient and robust performance of modern low-emission gas turbine combustor remains a challenge. The limitation of the experimental techniques to provide the detailed understanding of the physical problem strongly motivates the development of accurate computational techniques and models for predicting combustion behavior.

The main objective of this work is to deal with numerical modeling of turbulent reactive flows that are related to LP gas turbine combustion applications. The first goal is to implement, validate and improve the thickened flame LES models as an accurate methodology for simulating
premixed combustion. The second goal is to use this validated simulation tool to examine the effects of hydrogen addition on the overall premixed combustion behavior including the behavior of key metrics such as flashback, combustion dynamics, flame holding and emissions.

1.5 Outline of This Thesis

The thesis is organized in the following manner:

The present chapter provides an elaborate description on the background, motivation and objectives of this work.

Chapter 2 describes the mathematical description and modeling approaches for turbulent reactive flows. Firstly, it deals with the theoretical background of turbulence followed by the mathematical modeling and then discusses the physics and mathematics of the combustion in details.

Chapter 3 gives an overview of turbulent premixed combustion. It starts with the flame characteristics, and is then followed by the discussion on the regimes in turbulent premixed combustion. Finally, it describes different modeling techniques, especially for turbulent premixed combustion.

Chapter 4 mainly deals with the detailed description of Thickened Flame (TF) approach including different variants of this model. It also describes the proposed modified version of TF model and finally the derivation of the TF model in a LES framework.

Chapter 5 presents the numerical methods employed in this thesis work. It also discusses the details of the flow solver including the discretization scheme, boundary conditions, solution methodologies as well as the parallel communication.

Chapter 6 represents the validation studies of this computational approach. The validation of LES implementation has been studied for different flow configurations. As the first study, turbulent flow over a backward facing step for different Reynolds number has been simulated and compared the data with experiments. Then, the isothermal swirling flow in a confined geometry
has been studied and compared with experiments.

In chapter 7, LES of turbulent premixed combustion using the Thickened Flame (TF) approach has been examined on a Bunsen burner type geometry. Two sets of Reynolds numbers have been investigated in the context of detailed description of the flow fields. The effect of different chemistry models has also been explored in this chapter. The variants of TF model have been examined first and then the detailed results have been discussed based on original TF model and modified TF model in conjunction with 2 step chemistry.

Chapter 8 represents the natural gas combustion in an unconfined swirl stabilized burner. Firstly, it deals with the description of flow configuration, experimental techniques and computational details, and then followed by the non-reacting and reacting flow results in details.

In Chapter 9, the role of hydrogen addition in premixed combustion systems has been investigated in great details in the context of flame flashback. It provides an overview of swirling flow, mixing, and role of hydrogen addition in the context of gas turbine combustion. Finally, it emphasizes the issues pertaining to flashback due to hydrogen doping in premixed combustion systems.

Chapter 10 deals with the effects of swirl, geometry and premixedness in hyrodgen enriched premixed combustion systems. It mainly discusses the flame flashback behavior in the context of swirl, geometry, and boundary conditions in a combustor.

Chapter 11, the last chapter, concludes the current work, and provides a platform to the reader with the proposal for future work.

Appendix provides a glossary lists and nomenclature used in this dissertation.
Chapter 2 Mathematics: Turbulence and Combustion

This Chapter mostly deals with the different aspects of turbulence as well as combustion. To have a better understanding of the process, turbulent non-reactive flows are first discussed, followed by reactive flows.

2.1 Turbulence: Physics and Modeling

Turbulence, which is considered as probably the most significant unresolved problem in classical physics, yet to be fully understood, has importance in nearly all engineering applications. Turbulence is a state of fluid motion in which the instantaneous velocities exhibit random fluctuations.

2.1.1 Physics of Turbulence

It was almost a century ago, Osborne Reynolds first studied the transition to turbulence in a pipe flow. Finally, he came up with a non-dimensional parameter that is used to characterize the nature of the flow field. This dimensionless parameter is known as Reynolds number, defined as the ratio of inertia force to viscous force.

\[
Re = \frac{\rho UL}{\mu} = \frac{UL}{\nu}
\]

(2.1)

It is also a representation of convection term to diffusion term. Reynolds, in his experiment, found that the flow becomes turbulent after a critical value of Reynolds number which is around 2300 for a circular pipe. It is well known that, at high Reynolds number, the inertia forces become so dominant that viscous forces can no longer stabilize that and hence the flow becomes unstable. If the Reynolds number is high enough then the instability makes the flow to be turbulent in nature. Although, it is very difficult to define turbulence in a single word or single sentence, but
one can surely state the characteristics of a turbulent flow (Tennekes & Lumley, 1990) as follows:

- **Irregularity**
  
  All turbulent flows are irregular, or random in nature. This makes a deterministic approach to understand the turbulence problems impossible; instead, one relies on statistical methods.

- **Diffusivity**
  
  Another important feature of all turbulent flows is diffusivity that causes rapid mixing and increased rates of momentum, heat and mass transfer.

- **Large Reynolds Number**
  
  Turbulent flows always occur at high Reynolds number. Turbulence often originates as an instability of laminar flows if the Reynolds number become too large. The instabilities are related to the interaction of viscous terms and nonlinear inertia terms in the equation of motion.

- **Three-Dimensional Vorticity Fluctuations**
  
  Turbulence is rotational and three dimensional. Turbulence is characterized by high levels of fluctuating vorticity. For this reason, vorticity dynamics plays a essential role in the description of turbulent flows.

- **Dissipation**
  
  Turbulent flows are always dissipative. Viscous shear stresses perform deformation work which increases the internal energy of the fluid at the expense of kinetic energy of the turbulence. Turbulence needs a continuos supply of energy to make up their viscous losses.

- **Continuum**
  
  Turbulence is a continuum phenomenon, governed by the equations of fluid mechanics. Even the smallest scales occurring in a turbulent flow are ordinarily far larger than any molecular length scale.
• **Turbulent Flows are Flows**

Turbulence is not a feature of fluids but of fluid flows. Most of the dynamics of turbulence is the same in all fluids, whether they are liquids or gases, if the Reynolds number of the turbulence is large enough; the major characteristics of turbulent flows are not controlled by the molecular properties of the fluid in which the turbulence occurs.

Typically the turbulence properties are characterized with the occurrence of eddies of different scales. However, eddies are correlated with local value of velocity, length, time scale. In order to define the distribution of eddy length scales at any position, the velocities at point \((x, t)\) and point \((x+r, t)\) with a distance \(r\) apart from each other are measured simultaneously, and then the correlation between these two points is defined by the average

$$u'(x, t)u'(x + r, t)$$

the normalized correlation \(f(r; t)\) for a homogeneous isotropic turbulence is defined as

$$f(r, t) = \frac{u'(x, t)u'(x + r, t)}{\overline{u'(x, t)u'(x, t)}}$$

(2.2)

Figure 2.2 shows schematics of a normalized correlation \(f(r, t)\). It approaches unity for \(r \to 0\), but slowly decays if the distance between two points are very small. However, the distance increases then it may decrease continuously and may even take negative values. Moreover, when the eddy size becomes too large with a large distances between the two points, they do not contribute much to the correlation, however the occurrences are seldom though.

The phenomenological description of these eddies follows a nice hypothesis that there is an energy cascade from large scale to small turbulent scales as shown in Figure 2.1, which was first conjectured by Richardson in 1992 (Mathieu & Scott, 2000). Kolmogorov (1941) first proposed the energy cascade hypothesis for homogeneous isotropic turbulence. It assumes that there is a steady transfer of kinetic energy from the large scales to the small scales and this energy is being consumed at the small scales by viscous dissipation. The energy transfer rate, which is
Figure 2.1: Turbulent kinetic energy spectrum

independent of the size of the eddies within the inertial range, is defined as the production of kinetic energy $\kappa$ is equal to the dissipation rate $\epsilon$.

Within inertial subrange, extended from integral scale $l$ to Kolmogorov scale $\eta$, $\epsilon$ is the only dimensional quantity apart from the correlation coordinate $r$, is available for the scaling of $f(r,t)$.

The second order structure function defined as

$$F_2(r, t) = \overline{(u'(x, t) - u'(x + r, t))^2} = 2u'^2(t)(1 - f(r, t))$$  \hspace{1cm} (2.4)

which can be scaled as

$$F_2(r, t) = C(\epsilon r)^{2/3}$$  \hspace{1cm} (2.5)

where $C$ is the universal Kolmogorov constant. In the case of homogeneous isotropic turbulence, the turbulent kinetic energy ($\kappa$) is defined as

$$\kappa = \frac{1}{2} \overline{u'^2}$$  \hspace{1cm} (2.6)
is equal to $k = 3u'^2/2$. Using 2.4 and 2.5, it is found

$$f(r, t) = 1 - \frac{3}{4 \kappa} \frac{1}{(\varepsilon r)^{2/3}} \tag{2.7}$$

which is also shown in Figure 2.2. The eddies with characteristic size usually contain the most of the kinetic energy. At these eddies there remains a relative large correlation before it decays to zero. The length scale of these eddies is called the integral length scale $l$, which is defined as

$$l(t) = \int_0^\infty f(r, t)dr \tag{2.8}$$

The integral length is also shown in Figure 2.2. The root-mean square (r.m.s.) velocity and the integral times scale are defined as

$$u' = \sqrt{2\kappa/3} \tag{2.9}$$

$$\tau = \frac{\kappa}{\varepsilon} \tag{2.10}$$

In viscous subrange, the motion of these eddies are mostly influenced by viscosity, and turbulent kinetic energy is transformed into heat by viscous dissipation. Therefore, the kinematic viscosity, $\gamma (m^2/s)$, is considered as another dimensional quantity for scaling in addition to the dissipation rate, $\varepsilon (m^2/s^3)$. Hence, the characteristic length scale for this subrange, which is also known as Kolmogorov length scale $\eta$, time scale $t_\eta$ and velocity scale $u_\eta$, are determined through
dimensional analysis. The Kolmogorov length scale $\eta$, is also shown in Figure 2.2.

$$\eta = \left( \frac{\gamma^3 \epsilon}{\varepsilon} \right)^{1/4} ; t_\eta = \left( \frac{\gamma}{\varepsilon} \right)^{1/2} ; u_\eta = (\gamma \varepsilon)^{1/4} \quad (2.11)$$

The Taylor length scale is defined in between integral length scale and Kolmogorov scale. The average gradients in the definition of $\varepsilon$ (2.12) are replaced by $v'/\lambda$, which leads to

$$\varepsilon = \gamma \left[ \nabla v' + \nabla v'^T \right] : \nabla v' \quad (2.12)$$

$$\varepsilon = 15 \gamma \frac{v'^2}{\lambda^2} \quad (2.13)$$

where the factor 15 is originated from the assumption of isotropic homogeneous turbulence (Peters, 2000; Mathieu & Scott, 2000). The Taylor length scale, $\lambda$, is found to be proportional to $v' \eta$ using 2.13.

$$\lambda = \left( 15 \gamma v'^2 / \varepsilon \right)^{1/2} \sim v' t_\eta \quad (2.14)$$

Taylor length scale, $\lambda$, may also be interpreted as the distance that a large eddy convects a Kolmogorov eddy during its turnover time $t_\eta$.

According to Kolmogorov’s 1941 hypothesis the transferred energy from large eddies of integral length scale, $l$, is equal to the dissipation energy at the Kolmogorov scale $\eta$. Thus, the viscous dissipation ($\varepsilon$) can be estimated as

$$\varepsilon \sim \frac{v'^3}{l} \quad (2.15)$$

and also is independent of the size of the eddies within the inertial subrange. Hence, the discrete sequence of eddies are defined as (Peters, 2000)

$$l_n = \frac{l}{2^n} \approx \eta, n = 1, 2...$$

The kinetic energy spectrum $E(\kappa)$, which is the density of kinetic energy per unit wave-number $\kappa$, is obtained from the Fourier transform of the isotropic two-point correlation function. The wave-number $\kappa$ is related with the eddy size $l_n$ as

$$\kappa = l_n^{-1} \quad (2.16)$$
Then, the kinetic energy at the discrete scale \( l_n \) is estimated as
\[ \nu_n^2 \sim (\varepsilon l_n)^{2/3} = \varepsilon^{2/3} \kappa^{-2/3} \]  
(2.17)
the kinetic energy spectrum \( E(\kappa) \) is related with dissipation rate and wavenumber as
\[ E(\kappa) = \frac{d\nu^2_n}{d\kappa} \sim \varepsilon^{2/3} \kappa^{-5/3} \]  
(2.18)
This is the well-known \( \kappa^{-5/3} \) law for the kinetic energy spectrum in the inertial subrange. Figure
2.1 shows the typical plot (log-log) of energy spectrum for the entire range of wavenumber.
The large scale eddies are represented by small wave numbers, at which energy spectrum is not
universal and depend on the boundary conditions of the flow. The integral length scale where the
energy spectrum reaches the maximum, eddies contain most of the energy. As the wave-number is
further increased and falls into the inertial subrange, the energy spectrum decreases by following
the -5/3 law. There is a cutoff at the Kolmogorov scale \( \eta \), beyond that the range is known as
viscous subrange where the energy spectrum decreases exponentially owing to strong viscous
effects. By dimensional analysis, the relationship between integral scale and Kolmogorov scale is
found as
\[ \frac{l}{\eta} = \frac{\varepsilon^{1/4} l}{\gamma^{3/4}} \sim \frac{\nu'^{3/4} l}{\gamma^{3/4} l^{1/4}} \left( \frac{\nu' l}{\gamma} \right)^{3/4} = \text{Re}_l^{3/4} \]  
(2.19)
\[ \frac{\tau}{t_\eta} = \frac{l}{\nu'^t_\eta} = \frac{l \varepsilon^{1/2}}{\nu' \gamma^{1/2}} \sim \frac{l \nu'^{3/2}}{\nu' \gamma^{1/2} l^{1/2}} \left( \frac{\nu' l}{\gamma} \right)^{1/2} = \text{Re}_l^{1/2} \]  
(2.20)
\[ \frac{\nu'}{u_\eta} = \frac{\varepsilon^{1/4}}{\gamma^{1/4}} \sim \frac{\nu' l^{1/4}}{\gamma^{1/4} \nu'^{1/4}} \left( \frac{\nu' l}{\gamma} \right)^{1/4} = \text{Re}_l^{1/4} \]  
(2.21)
Where \( \text{Re}_l = \nu' l / \gamma \) is so called turbulent Reynolds number defined at the integral scale. The
Taylor length scale and integral length scale can also be correlated (using 2.14) as
\[ \frac{l}{\lambda} \sim \frac{l}{\nu'^t_\eta} = \frac{l}{\nu' \eta} \sim \text{Re}_l^{3/4} \text{Re}_l^{-1/4} = \text{Re}_l^{1/2} \]  
(2.22)

2.1.2 Reynolds Averaged Navier-Stokes Equation(RANS) Modeling

The statistical methods seem to be more useful to predict the turbulent flow due its randomness
in nature. Reynolds averaged Navier-Stokes (RANS) equations is one of the classical approaches extensively used in industrial applications over a long period of time. The main philosophy behind RANS is to do single point averaging of the Navier-Stokes equations and decompose the turbulent variables into mean and fluctuating value.

In order to obtain the mean value, there are several methods available and used, such as time averaging, space averaging, ensemble averaging and weighted averaging. The concept of time-averaging is that each instantaneous variable of the system (e.g. $\phi$) is decomposed in two parts: a mean part usually denoted with $\bar{\phi}$, and a fluctuating part $\phi'$:

$$\phi = \bar{\phi} + \phi'$$  \hspace{1cm} (2.23)

In RANS models, it is assumed that there exist a time separation between the fluctuating time scales ($t_1$) and the main time scale ($t_2$, characteristic of the "slow" variation of mean flow) and they differ by several orders of magnitude ($t_1 << t_2$), otherwise the mean and fluctuation components would not be uncorrelated. With the assumption of "short-time" averaging for a time dependent variables, for a period of $\Delta t$ which $t_1 < \Delta t < t_2$, the time averaged variable is defined as:

$$\bar{\phi}(\vec{r}, t) = \overline{\phi} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \phi(\vec{r}, t')dt'$$  \hspace{1cm} (2.24)

The mean of the fluctuating part is set to zero, according to

$$\overrightarrow{\phi'} = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left( \phi(\vec{r}, t') - \bar{\phi}(\vec{r}, t') \right) dt'$$

$$= \overline{\phi(\vec{r}, t')} - \bar{\phi}(\vec{r}, t') \equiv 0$$  \hspace{1cm} (2.25)

Large density variations are typically found in combustion processes or compressible flows, where the implementation of time averaging method to the Navier-Stokes equations makes arise of some terms containing $\rho'$, such as $\rho'u'$. As a consequence, the classical approach of modeling turbulent flows with time averaging techniques is extended to include density variation effects by introducing density-weighted averages (so called Favre averaging). This kind of averaging allows much more compact formulation with fewer unknown correlations in the process of deducing the
averaged Navier-Stokes equations. The Favre averaging of a variable \( \phi \) is defined as:

\[
\overline{\phi} = \frac{\rho \bar{\phi}}{\bar{\rho}}
\]

(2.26)

Then the decomposition of the variable \( \phi \) can be written in same manner as :

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

(2.27)

where \( \bar{\phi} \) is the Favre averaged mean value, and \( \phi'' \) is the fluctuating term. From the definition, it is found that

\[
\overline{\rho \phi} = \rho(\phi - \phi'') = \overline{\bar{\phi}} + \overline{\rho \phi''} = \overline{\rho \bar{\phi}} + \overline{\rho \phi''}
\]

(2.28)

and

\[
\overline{\rho \phi''} = \rho(\phi - \bar{\phi}) = \overline{\rho \bar{\phi}} - \overline{\rho \phi} = \overline{\rho \bar{\phi}} - \overline{\rho \bar{\phi}} \equiv 0
\]

(2.29)

The Favre averaging requires the density as a factor to weight the variable :

\[
\overline{\rho(\vec{r}, t) \phi(\vec{r}, t)} = \overline{\bar{\rho}} \overline{\bar{\phi}} = \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} \rho(\vec{r}, t') \phi(\vec{r}, t') dt'
\]

(2.30)

where

\[
\overline{\rho(\vec{r}, t)} = \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} \rho(\vec{r}, t') dt'
\]

(2.31)

For variable density flows, the governing equations in conservative form are written as :

\[
\text{Continuity :} \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0
\]

(2.32)

\[
\text{Momentum :} \quad \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}
\]

(2.33)

where \( \tau_{ij} \) is the viscous tensor, defined as

\[
\tau_{ij} = \mu \left( 2 S_{ij} - 2/3 \delta_{ij} \frac{\partial u_k}{\partial x_k} \right)
\]

(2.34)

\( S_{ij} \) is the strain rate tensor is given by

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

(2.35)

Applying the Favre averaging on 2.32 and 2.33, we obtain

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

(2.36)
\[
\frac{\partial \rho \bar{u}_i}{\partial t} + \frac{\partial \rho \bar{u}_i \bar{u}_j}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \rho \bar{u}_i \bar{u}_j' \right)
\]  
(2.37)

where \( \tau_{ij} \) and \( \bar{\tilde{S}}_{ij} \) are the averaged viscous tensor and strain rate tensor, respectively, given as:

\[
\bar{\tau}_{ij} = \mu \left( 2 \bar{\tilde{S}}_{ij} - 2/3 \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \right)
\]  
(2.38)

\[
\bar{\tilde{S}}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]  
(2.39)

The averaged continuity equation 2.36 looks exactly similar to the original one 2.32, however, the averaged momentum equation 2.37 is differ from the original one 2.33 by an unclosed correlation term, \(-\rho \bar{u}_i'' \bar{u}_j''\), needs to be modeled, is known as Reynolds stress tensor.

The simplest turbulence models are largely based on the Boussinesq eddy-viscosity hypothesis. The modeling of Reynolds stress as proposed by Boussinesq is the product of an equivalent turbulent eddy viscosity \( \mu_t \), and the mean strain rate tensor, leads rise to the calculation of eddy viscosity \( \mu_t \).

\[
-\rho \bar{u}_i'' \bar{u}_j'' = \mu_t \left( 2 \bar{\tilde{S}}_{ij} - 2/3 \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \right) - 2/3 \delta_{ij} \rho \kappa
\]  
(2.40)

The last term is required in order to fulfill \(-\rho \bar{u}_i'' \bar{u}_j'' = -2\rho \kappa \).

There are inherent drawbacks in the models which are originated from Boussinesq eddy-viscosity hypothesis (Wilcox, 1998). First of all, modeled Reynold stress strictly follows the mean strain rate change without any delay, means history effect is not taken into account. Secondly, it does not account for the extra strain rates which are produced due to rotational movement, which is an antisymmetric tensor \( \bar{\Omega}_{ij} \), whereas \( \bar{\tilde{S}}_{ij} \) is a symmetric tensor. \( \bar{\Omega}_{ij} \) is defined as:

\[
\bar{\Omega}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]  
(2.41)

Due to the above-mentioned reasons, the turbulence models based on the Boussinesq hypothesis are not found to be suitable (Wilcox, 1998) for: flow over curved surfaces, flow with sudden changes in mean strain rate, flow with rotation or swirl, flow in ducts with secondary motions,
flow with boundary layer separation, and in general non-isotropic flows.

However, the models based on Boussinesq hypothesis are widely used though, inspite of having many drawbacks. The reason behind that it is simple enough, easy to implement, and computationally inexpensive compared to the large eddy simulation (LES) and direct numerical simulation (DNS). The main attention of many Boussinesq hypothesis based models is to estimate the turbulent eddy- viscosity $\mu_t$, appeared in 2.40. The dimensional analysis shows that the $\mu_t$ can be calculated as

$$ \mu_t = C_{\mu} \overline{u^*} l^* $$

(2.42)

where $C_{\mu}$ is a constant, $u^*$ is a turbulent velocity scale and $l^*$ is a turbulent length scale.

- **Zero-equation Model**

  These models are known as algebraic model. Basically, some algebraic expressions are used to calculate $\mu_t$, hence no transport equation is needed. The use of these models are very limited, like jet flows, mixing layer flows. Prandtl mixing length model (Prandtl, 1925), Cebeci-Smith model (Smith & Cebeci 1967), and Baldwin-Lomax model (Bldwin & Lomax, 1978) are the examples of these type of model.

- **One-equation Model**

  A more general formulation of this kind of model solves a transport equation, usually the turbulent kinetic energy $\kappa$, and the other turbulent scale is estimated using some algebraic relation. The $\mu_t$ is then modeled as:

$$ \mu_t = C_{\mu} \overline{\rho} \sqrt{\kappa} l^* $$

Most of the applications solved using this kind of model only exhibited modest differences compared to the zero equation model, hence, not very commonly used (Wilcox, 1998). The examples of this kind of models are Baldwin-Barth model (Bldwin & Barth, 1990) and Spalart-Allmaras model(Spalart & Allmaras 1992).
• Two-equation Model

In this kind of model, two separate transport equations (turbulent kinetic energy and its dissipation) are solved to estimate $\mu_t$. Compared to zero or one equation model, it can be used to calculate any turbulent flow without having a prior knowledge of the turbulent structure. The two transport equations are having many closure coefficients which vary from case to case and need to be tuned properly. There are different type of two-equation models have been developed based on the closure approximation of $\mu_t$. For example, $\kappa - \omega$ ((Kolmogorov, 1942), (Lauder & Spalding, 1972)) model, $\kappa - \tau$ ((Speziale et. al. 1990) ) model, $\kappa - \varepsilon$ ((Jones & Launder, 1972), (Lauder & Sharma, 1974)) model are different type of two-equation models.

A two-equation ($\kappa - \varepsilon$) model for reacting flows was proposed by Jones and Whitelaw (1982) as :

$$\frac{\partial \rho \kappa}{\partial t} + \frac{\partial \rho \bar{u}_j \kappa}{\partial x_j} = -\frac{\mu_t}{\rho} \frac{\partial \rho}{\partial x_i} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \left( \mu + \frac{\mu_t}{Pr_\kappa} \right) \frac{\partial \kappa}{\partial x_j} \right) - \left( \frac{\bar{p} \bar{u}_i \bar{u}_j}{\varepsilon} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \bar{p} \varepsilon$$

(2.43)

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho \bar{u}_j \varepsilon}{\partial x_j} = -C_{\varepsilon 1} \frac{\varepsilon}{\kappa} \left( \frac{\mu_t}{\rho^2} \frac{\partial \rho}{\partial x_i} \frac{\partial \bar{p}}{\partial x_i} \right) + \frac{\partial}{\partial x_j} \left( \left( \mu + \frac{\mu_t}{Pr_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) - C_{\varepsilon 2} \frac{\varepsilon^2}{\kappa}$$

(2.44)

Where the model constants are $Pr_\kappa=1.0$, $Pr_\varepsilon=1.3$, $C_{\varepsilon 1}=1.44$, $C_{\varepsilon 2}=1.92$. These coefficients are proposed based on experiments. The turbulent eddy-viscosity is then approximated as :

$$\mu_t = C_\mu \frac{\rho \varepsilon^2}{\varepsilon}$$

(2.45)

where $C_\mu=0.09$.

• Reynolds Stress Model (RSM)

Six components of Reynold stress tensor are solved through separate transport equations. However, there are 22 new unknowns show up in the derived six new equations (Wilcox, 1998), and all of these unknown terms need to be modeled in some way (Lauder et. al. 1975). RSM has few advantages over Boussinesq hypothesis based RANS models, because it automatically
accounts for the convection and diffusion of Reynolds stress tensor, effects of streamline curvature, system rotation, and so on. Due to complexity and computational difficulty, RSM is not widely used yet, though it gives a more complete description of the physics.

Additionally, the nonlinear algebraic constitutive relationship are available (Wilcox, 1998) to overcome the drawbacks of standard Boussinesq hypothesis based RANS models. Wilcox and Rubesin (1980) proposed a nonlinear relationship for their \( \kappa - \omega^2 \) model,

\[
-\rho u_i u_j = \mu_t \left( 2\tilde{S}_{ij} - 2/3\delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right) - 2/3\delta_{ij} \tilde{p} \kappa + \frac{8}{9} \rho \kappa \left( \tilde{S}_{ik} \Omega_{kj} + \tilde{S}_{jk} \Omega_{ki} \right) + \frac{8}{9} \rho \kappa \left( \beta \omega^2 + 2\tilde{S}_{mn} \tilde{S}_{nm} \right)
\]  

(2.46)

Rodi (1976) derived a nonlinear constitutive relation from the full RSM equations after simplification, which is also known as algebraic stress model (ASM or ARSM). Johansson et al. (1996) came up with an explicit algebraic Reynolds stress model (EARSM), moreover, few more developments have been proposed in Wallin and Johansson (2000).

2.1.3 Large Eddy Simulation (LES)

The central idea behind large eddy simulation (LES) is to explicitly compute the large scale structures of the flow field (typically structures larger than the computational mesh size) whereas the effect of the smallest ones are modeled. LES is an intermediate approach between RANS and DNS, though it has several advantages over the RANS models. Small eddies are the less energy carrying structures and having more universal and isotropic features. Modeling of small eddies are relatively easier than to model the full spectrum. The higher energy carrying structures or large eddies, which are mostly affected by the flow geometry and boundary conditions, represent the time-dependent unsteady flow behavior of the flow.

In LES, the variables are filtered in spectral space (eddies with greater frequency than the cut-off frequency are suppressed) or in physical space (weighted average over a given volume). The detailed information on filtering and filter functions are found in Piomelli (1999). The discussion on spacial filtering is carried out here. In space filtering, filter function \( F \) with the filter
width $\Delta$ is applied to a flow variable $\phi$ to obtain a filtered flow variable $\overline{\phi}$, by

$$
\overline{\phi}(x, t; \Delta) = \int_{-\infty}^{+\infty} F(x - x'; \Delta) \phi(x', t; \Delta) dx'
$$

(2.47)

The filter function F must satisfy the normalization condition

$$
\int_{-\infty}^{+\infty} F(x - x'; \Delta) dx' = 1
$$

(2.48)

Like RANS the flow variable is decomposed into two parts: resolved ($\overline{\phi}$) and unresolved part ($\phi'$)

$\phi = \overline{\phi} + \phi'$. However, LES filtering properties differ from RANS though. Here, the filtered unresolved component is not zero, like $\overline{\phi'} \neq 0$, and $\overline{\phi} \neq \overline{\phi}$. For Favre filtering also: $\phi = \overline{\phi} + \phi''$, $\overline{\phi'} \neq 0$, and $\overline{\phi} \neq \overline{\phi}$.

Applying the filtering technique on the equations 2.32 and 2.33, the equations take the following form

$$
\frac{\partial \overline{p}}{\partial t} + \frac{\partial \overline{p} \overline{u}_j}{\partial x_j} = 0
$$

(2.49)

$$
\frac{\partial \overline{p} \overline{u}_i}{\partial t} + \frac{\partial \overline{p} \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j} (\overline{p} \overline{u}_i \overline{u}_j - \overline{\rho} \overline{u}_i \overline{u}_j)
$$

(2.50)

where $\tau_{ij}$ is the viscous tensor, has the similar form as 2.38. The term $T_{ij} = \overline{p} \overline{u}_i \overline{u}_j - \overline{\rho} \overline{u}_i \overline{u}_j$ is an unclosed term, and traditionally, is known or called as subgrid scale (SGS) stress tensor. Chow and Moin (2003), Katopodes et al. (2000) proposed this term as subfilter scale (SFS), because the smallest eddy scale is always in the order of filter scale and larger than grid size. However, the traditional name, SGS, has been followed here. There are different SGS model are found in literature. Piomelli (1999) summarized the main models developed till today. The main role of SGS model is to dissipate the energy transferred from large scales, since the viscous subrange in the turbulent kinetic energy spectrum are usually un resolved (Piomelli, 1999). The commonly used SGS models are briefly discussed below.

- **Smagorinsky Model**

Smagorinsky model is one of the most popular models because of its simple formulation
(Smagorinsky, 1963). It is based on the large scales and the unresolved term is modeled based on Boussinesq assumption as

\[ T_{ij} - \frac{\delta_{ij}}{3} T_{kk} = -\nu_t \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) = -2\nu_t \tilde{S}_{ij} \]  

(2.51)

Where \( \tilde{S}_{ij} \) is the filtered strain rate tensor. The eddy-viscosity is the calculated as

\[ \nu_t = (C_s \Delta)^2 \left\| \tilde{S} \right\| = (C_s \Delta)^2 \left( 2\tilde{S}_{ij} \tilde{S}_{ij} \right)^{1/2} \]  

(2.52)

Where \( C_s \) is a model constant, \( \Delta \) is filter size. For homogeneous isotropic turbulence, the model constant is proposed as \( C_s \approx 0.2 \). The main problem with model is that the value of the model constant is not generic, and needs to be tuned from case to case. Moreover, this model is known as being too much dissipative, especially near walls. In addition to that, this model does not take care the back-scatter phenomenon which become really important in transition problems (Lesieur & Métais, 1996; Maneuveau & Katz, 2000).

- **Scale Similarity Model (SSM)**

Bardina et al. (1980) proposed this model. It is based on the assumption that the unresolved stresses play a major role due to those largest unresolved eddies, similar to the smallest resolved eddies. The smallest scale contribution can be estimated by applying filtering process on the resolved scales. The expression for this model is

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

(2.53)

This model was found to be insufficiently dissipative, so Bardina et al. (1980) proposed the idea of mixed model which is derived by coupling Smagorinsky model with SSM. Liu et al. (1994) came up with a different model which is a coupled model of Smagorinski model and SSM model with a second filtering function. This model is expressed as

\[ T_{ij} = C_L \bar{p} \left( \tilde{u}_i \tilde{u}_j - \bar{p} \tilde{u}_i \tilde{u}_j \right) - \bar{p}(C_s \Delta)^2 \left( 2\tilde{S}_{ij} \tilde{S}_{ij} \right)^{1/2} \tilde{S}_{ij} \]  

(2.54)

Wang et al. (2004a; 2005) and Gullbrand et al. (2001) used the dissipative nature of numerical scheme in 2.54 to get rid of the excessive dissipativity of the Smagorinsky model.
**Germano Dynamic Model**

Germano et al. (1991) proposed a dynamic SGS model is to estimate small scale dissipation form the knowledge of resolved scales to improve the Smagorinsky model. In the dynamic model, the model constant is automatically calculated during the simulations depending on time and space without assuming pre-determined constant anymore. The SGS stress tensor \( T_{ij} = \overline{p\tilde{u}_i\tilde{u}_j} - \overline{p\tilde{u}_i\tilde{u}_j} \) can be modeled as

\[
T_{ij} - \frac{\delta_{ij}}{3} T_{kk} = C \alpha_{ij} \tag{2.55}
\]

Where \( C \) is a model parameter and \( \alpha_{ij} \) needs to be modeled. Applying a second filtering operation on the filtered momentum equation 2.50, a similar term for sub-test-scale tensor (STS) is obtained and defined as \( \Upsilon_{ij} = \overline{\overline{p\tilde{u}_i\tilde{u}_j}} - \overline{p\tilde{u}_i\tilde{u}_j} \). It can be modeled in similar fashion as

\[
\Upsilon_{ij} - \frac{\delta_{ij}}{3} \Upsilon_{kk} = C \beta_{ij} \tag{2.56}
\]

where \( \beta_{ij} \) needs to be modeled too. Germano et al. (1991) estimated the Reynold stresses \( T_{ij} \) and \( \Upsilon_{ij} \) from the Smagorinsky model as

\[
\alpha_{ij} = -2\overline{\overline{\rho\Delta^2}} \left( \overline{\overline{S_{mn}S_{mn}}} \right)^{1/2} \overline{S_{ij}} \tag{2.57}
\]

\[
\beta_{ij} = -2\overline{\overline{\rho\Delta^2}} \left( \overline{\overline{S_{mn}S_{mn}}} \right)^{1/2} \overline{\overline{S_{ij}}} \tag{2.58}
\]

Germano identity is written as

\[
L_{ij} = \overline{\overline{p\tilde{u}_i\tilde{u}_j}} - \overline{\overline{p\tilde{u}_i\tilde{u}_j}} = \Upsilon_{ij} - \overline{T_{ij}} \tag{2.59}
\]

where \( L_{ij} \) can be rewritten using the expression of \( \alpha_{ij} \) and \( \beta_{ij} \),

\[
L_{ij} - \frac{\delta_{ij}}{3} L_{kk} = C \left( \beta_{ij} - \overline{\alpha_{ij}} \right) \tag{2.60}
\]

This equation system contain six equations with one unknown, essentially become a over defined system. Using least square technique, the parameter \( C \) is determined. The error is defined as

\[
Q = \left( L_{ij} - \frac{\delta_{ij}}{3} L_{kk} + CM_{ij} \right)^2 \tag{2.61}
\]

where \( M_{ij} = (\overline{\alpha_{ij}} - \beta_{ij}) \). The minimum error corresponds to \( \partial Q / \partial C = 0 \). After simplification of
the algebra, $C$ is obtained as
\[
C = -\frac{L_{ij}M_{ij}}{M_{ik}M_{lk}}
\]  
(2.62)

Dynamic model found to be very efficient for different class of problems without making any *ad-hoc* assumption for the model constant $C$, which is calculated during simulations depending on the flow physics. Moin et al. (1991) used dynamic model to simulate compressible flows and scalar transport problem.

**2.1.4 Detached Eddy Simulation (DES)**

Detached-Eddy Simulation was first proposed by Spalart et al. (1997) to predict the turbulent flows at high Reynolds number. It is a hybrid technique, which has RANS behavior near the solid surfaces and LES behavior away from solid surfaces. The computational cost for doing complete LES simulations for the configurations like airplane, submarine with appropriate boundary layer resolution, motivated the development of this technique. The main idea behind DES is to combine the most favorable aspects of the two techniques, i.e., application of RANS models for predicting the attached boundary layers and LES for resolution of time-dependent, three-dimensional large scale structures with minimum modeling. Hence, the DES becomes very much cost effective technique due to that fact the LES is not applied to resolution of the relatively smaller-structures that populate the boundary layer. So far, it has not been extensively used in combustion calculations.

**2.1.5 Direct Numerical Simulation (DNS)**

DNS is a complete numerical simulation of three-dimensional balance equations without any turbulence models. In order to capture the turbulence features of the flow field, it is necessary to resolve the length and time scale of turbulence properly. Essentially, the computational grid needs to be fine enough, and time step as well in the limit of Kolmogorov length and time scale. The capability of DNS has become promising in combustion studies for investigating the flame-turbulence interaction and significant progress has been achieved so far (Givi, 1989, 1994;
Poinset & Veynante, 2001). Nevertheless, DNS, being a promising tool, has few drawbacks. DNS calculations need huge computational resources and high order discretization schemes to reduce the numerical error in the solution. Till today, DNS has been successfully applied to flows with moderate Reynolds numbers and simple geometry.

2.2 Combustion: Theory and Modeling

2.2.1 Mathematical Description of Combustion

Combustion is a process where fuels are burned into combustion products due to presence of air. There are many species and chemical reactions are involved in a combustion process. The basis of any combustion model is the continuum formulation of the balance equations for energy as well as chemical species. The system of species transport equations are solved in addition to the Navier-Stokes equations for the flow field. Given the mass fraction of species \( i \) as \( Y_i \) \((i = 1, 2, ..., n)\), where \( n \) is the number of species involved in chemical reactions, the transport equation for species \( i \) is defined as:

\[
\frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho Y_i u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( D_{ij} \frac{\partial Y_j}{\partial x_i} \right) + \omega_i \tag{2.63}
\]

where \( \omega_i \) is the formation rate of species \( i \) or chemical source term, \( D_{ij} \) is the binary mass diffusion coefficient, or mass diffusivity of species \( i \). The chemical source term \( \omega_i \), which is the mass of species \( i \) produced per unit volume and unit time, is the sum over all reactions involved in the mechanism:

\[
\omega_i = W_i \sum_{k=1}^{r} \gamma_{ik} \omega_{ik} \tag{2.64}
\]

where \( \gamma_{ik} = \gamma_{ik}^{+} - \gamma_{ik}^{-} \). Essentially, sum over all source term must vanishes, \( \sum_{k=1}^{r} \omega_i = 0 \).

The rate of reaction \( (\omega_k) \) in a mechanism containing \( r \) chemical reactions is defined as

\[
\omega_k = k_{fk} \prod_{j=1}^{n} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{ik}^{+}} - k_{bk} \prod_{j=1}^{n} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{ik}^{-}} \tag{2.65}
\]

where \( W_j \) is the molecular weight of species \( i \), \( k_{fk} \) and \( k_{bk} \) are the rate coefficients of the forward and backward reaction, respectively. The exponents \( \gamma_{ik}^{+} \) and \( \gamma_{ik}^{-} \) are the stoichiometric
coefficients of reaction $k$ in forward and backward direction, respectively. The reaction rate coefficients are temperature dependent, and usually calculated using the empirical Arrhenius expression (Poinsot & Veynante, 2001):

$$k_{f_k} = A_{f_k} T^b \exp \left( -\frac{E_k}{RT} \right)$$

(2.66)

where $A_{f_k}$, $b$, $E_k$ and $R$ are pre-exponential coefficient, temperature exponent, activation energy and universal gas constant, respectively. The backward reaction rates $k_{b_k}$ are calculated from the forward rates through equilibrium constants:

$$k_{b_k} = \frac{k_{f_k}}{\left( \frac{p_a}{RT} \right) \sum_{k=1}^{K} \gamma_k \exp \left( \frac{\Delta S_k^o}{R} - \frac{\Delta H_k^o}{RT} \right)}$$

(2.67)

where $p_a=1$ bar, and the $\Delta$ refers to the changes occurring when passing from reactants to products in $k^{th}$ reaction : $\Delta H_k^o$ and $\Delta S_k^o$ are the enthalpy and entropy changes for reaction $k$, respectively. These quantities are obtained from tabulation or the given chemical reaction mechanisms. In the species transport equation 2.63, the diffusive flux in the first term on the r.h.s. of that equation, is based on Fick’s law.

### 2.2.2 Modeling Approaches and Reaction Rate Modeling

The mean heat release rate is one of the main quantities of practical interest which needs to be calculated properly. The simplest or most direct way of doing so is to use Arrhenius expression or some Taylor series expansion of the same. Although, the species, reactions and chemical kinetics parameters need to be known before doing the calculation. The fact of matter is that this information is mostly obtained experimentally and there has been an ongoing disputes in kinetics community regarding the values of the kinetic parameters which have been developed and need to be developed and updated more over a period of time (Just, 1994). Considering the simple example of Methane reaction mechanisms: it consisted of less than 15 elementary reactions with 12 species in the period around 1970s, whereas it has been evolved to 53 species and 325 elementary reactions in the GRI mechanism (http://me.berkeley.edu/ gri_mech/). In case of more
complex fuel, the numbers of the species and elementary reactions are even more, effectively it leads to the requirement of huge computational resources for taking the full kinetics into account. Usually, in order to study flame structures, ignition and extinction conditions, instabilities, the full kinetics are taken into consideration. However, the affordability of doing detailed numerical modeling (DMM) is strictly limited to very simple flow configurations, such as plane, cylindrical or spherical flames. Mostly, DNM is used to create the flamelet libraries or test database for many turbulent combustion models by reducing complex reaction mechanisms.

There are different ways of resolving the problem, however, one most common way to solve this problem is to simplify the kinetic mechanism by keeping the important part of the chemical information intact. For example, a four-step global reduced mechanism for methane-air combustion system is proposed (Peters, 1985) by using steady state and partial equilibrium assumptions. By assuming the radial H is in steady state, this four-step mechanism is further reduced to three steps (Peters & Williams, 1987). Later on, by introducing the steady state assumption for H2, Bui-Pham et al. (1992) developed a two-steps mechanism. The main advantages of these reduced mechanisms are the dramatic enhancement in computational efficiency and good enough predictions for burning velocity, flame structure, as well. Mauss et al. (1993a; 1993b) and Løvás et al. (2000; 2002) did similar kind of analysis for hydrogen flames and hydrocarbon fuels. Jones and Lindstedt (1988) proposed a four-step reaction mechanism for the combustion of alkane hydrocarbons (up to butane) based on the flame structure analysis. More rigorous information on mechanism reduction can be found in Westbrook and Dryer (1981), Peters (1985), and Seshadri (1996).

DNS of turbulent combustion still remains a challenge in the context of computational resources and complex flame-turbulence interactions, even after having all these reduced reaction mechanisms developed. In addition to turbulent length and time scales, the reaction/flame length
and time scales need to be accounted for DNS calculation, which makes the accessible range for DNS of turbulent combustion not to be only dependent on the Reynolds number but also on other parameter in combustion, such as the Damköhler number. Numerous and detailed studies on DNS of turbulent premixed and non-premixed combustion, have been conducted by several researchers and can be found in Poinset et al. (1996), Candel et al. (1999), and Vervisch and Poinset (1998). Presently, DNS is used to study flame-turbulence interaction for betterment of turbulence combustion models, because most of the DNS calculations only resolve the turbulent scales and handle the other scales, associated with the flame, by using some simplified models, such as use of simple chemical mechanism and simple transport schemes. DNS is used to study flame quenching and the flame-vortex interaction (Poinset et al., 1991, 1990). Domingo and Vervisch (1996) also studied the important edge-flame (or the so-called triple flame) phenomenon using DNS.

Despite of having advancement in reduced kinetic mechanisms, it is obvious to keep the important fact in mind that any reduced reaction mechanism is only faithful to the full mechanism over a limited range of conditions, which may vary in the real combustion conditions (e.g. temperature, composition) in both space and time. One advancement was made by Schwer et al. (2003) where they used some adaptive reaction method, in which several reduced reaction mechanism are used in the same simulation. However, only one suitable reduced model (suitable to local conditions) is used locally with a hope to reproduce the full chemistry accurately without using too much computational resources. Moreover, the key challenge remains in understanding the utilization of appropriate adaptive chemistry models for different conditions within the flame as well as the definition of feasible criteria for switching between chemistry models.

Schwer et al. (2003) studied two simple flames. One of them is the H2/O2 shear layer diffusion flame consisting a full reaction mechanism with 12 species and 23 reactions. In order to account
for the hydrogen-rich and oxygen-rich conditions, two different reduced models are derived which are only valid below temperature 1500 K. In addition to that pure H2/N2 and O2/N2 models without reaction are also used. The switching criteria are defined based on the temperature and the hydrogen and oxygen mass fractions. It is evident from their studies that the large areas in the domain are computed using reduced models effectively, the necessity of the full mechanism is rather restricted only in a small region around the shear layer. A quite a bit good agreement is found between the full chemistry and adaptive chemistry solutions. It is believed that more complex combustion cases can be efficiently handled by using adaptive chemistry, which almost saves 60% CPU time.

- **Averaged Governing Equation**

Applying Favre averaging to the species transport equation 2.63,

\[
\frac{\partial \rho \tilde{Y}_i}{\partial t} + \frac{\partial \rho \tilde{Y}_i \tilde{u}_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{D}_i \rho \frac{\partial \tilde{Y}_i}{\partial x} \right) + \tilde{\omega}_i - \frac{\partial}{\partial x_i} \left[ \rho \left( \tilde{Y}_i \tilde{u}_i - \tilde{Y}_i \tilde{u}_i \right) \right]
\]  

(2.68)

where the first term on r.h.s. is molecular diffusion flux, and \( \tilde{\omega}_i \) is the mean chemical source term. The last term on r.h.s. is unresolved scalar fluxes due to turbulent transport. The unresolved turbulent transport term is generally modeled with a simple classical gradient assumption (Peters, 2000),

\[
\tilde{\rho} \left( \tilde{Y}_i \tilde{u}_i - \tilde{Y}_i \tilde{u}_i \right) = - \frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}_i}{\partial x_i}
\]

(2.69)

where \( \mu_t \) is the turbulent eddy viscosity and \( Sc_t \) is turbulent Schmidt number. This idea of gradient transport assumption is originally inferred from the turbulent scalar transport models in non-reactive, constant density flows. Sufficient numerical stability is obtained due to the diffusive nature of the modeled term. Bray et al. (1981) and Shepherd et al. (1982) showed that there exist a counter gradient scalar turbulent transport in some flames through experiment and theoretical study as well. The countergradient transport is taken place due to the differential effect of pressure gradients on cold reactants and hot products, and gas expansion effect.
However, the modeling of mean reaction source term is a challenging task in turbulent combustion. As the reaction rate term is highly non-linear (2.66) in nature, the averaged mean reaction rate ($\bar{\tau}$) can not be easily expressed as a function of species mass fraction ($\tilde{Y}_i$), mean density ($\bar{\rho}$) and the mean temperature ($\tilde{T}$), leading to main source of difficulties associated with turbulent combustion modeling. Several researcher (Jones and Whitelaw (1982), Candel et al. (1999)) addressed this problem and finally came up with an idea of modeling this specific term based on physical analysis. There are mainly three types of analytic concepts exist (Veynante, 2002).

(1) Turbulent Mixing Models

In this type of analysis, the assumption is that the reaction is too fast and the turbulent time scales are larger than reaction times scales (large Damköhler number), hence the reaction rate is mainly controlled by turbulent mixing rates. The turbulent mixing rates are generally expressed in terms of scalar dissipation rates. The simple popular models, i.e. eddy-break-up (EBU) model and eddy-dissipation-concept (EDC) model, belong to this family.

(2) Statistical Models

A system of joint probability density function (pdf) transport equations for the velocity and the reactive scalars are solved in this type of analysis. The idea behind this analysis is that for a given statistical properties of scalar fields at any location in the flowfield, their mean values and correlations can be extracted. Any complex reaction mechanisms can be handled in this type of analysis without having much difficulties, because the chemical reaction term is closed and no modeling is required. Monte-Carlo simulation techniques, which was proposed by Pope (1985), used to solve the system of equations due to high dimensionality. The pdf models are usually classified into two categories, i.e. presumed pdf and transport equation for the pdf. The conditional moment closure (CMC) model and the Bray-Moss-Libby (BML) model fall into this
kind of analysis.

(3) Geometrical Analysis Based Models

The flame front is generally viewed as a geometrical surface which is evolved in turbulent flow field. In usual notation, this surface is defined as an instantaneous iso-surface of mixture fraction for non-premixed flame or iso-surface of mass fraction/progress variable or G scalar for premixed flame. This method is based on flamelet assumption, in which each flame element is assumed to behave as a laminar flame. As the chemical mechanism is decoupled from the turbulent flow field, makes this one an advantageous approach. G-equation based analysis in one of the popular example of this type of approach (Peters, 1999; Nilsson & Bai, 2002; Wang & Bai, 2004b).

2.2.3 Premixed and Non-premixed Turbulent Combustion Modeling

In non-premixed combustion, which is commonly known as diffusion type combustion, the reaction is concentrated into a narrow flame zone at the stoichiometric state surface that separates the fuel and air. The fuel and air is mixed first (due to diffusion and turbulence) and then the reaction takes place. The fast chemistry assumption is strictly followed here, since the time needed for convection and diffusion is much larger than the time needed for reaction to occur (mainly diffusion controlled reaction rates), which introduces a significant simplification (Peters, 2000). Contrarily, in premixed combustion, as the mixing process is already been taken care of, the chemical kinetics becomes very important and dominant. Moreover, the flame thickness of premixed combustion is usually thinner than that of non-premixed flame, in fact, it is also usually smaller than the Kolmogorov length scale. Reynolds number and Damköhler number play a major role in deciding the influence of mixing or chemistry on reaction rates, so makes this type of combustion more difficult to model.

Additionally, 'conserved scalar' variable, known as mixture fraction, can be introduced into the non-premixed combustion modeling. Mixture fraction transport equation does not have any reaction source term, so makes it easier to implement just like N-S equations, and rest of the all
scalars such as temperature, species concentrations, and density are related to this variable in some algebraic way. Bilger (1993) and Klimenko (1990) proposed a conditional moment closure (CMC) concept for non-premixed turbulent combustion. Their observation also showed that the fluctuation of mixture fraction can directly be associated with fluctuation of the reactive scalars. Unfortunately, this variable is not useful for premixed combustion modeling due its constant value everywhere in the flow field.
Chapter 3 Turbulent Premixed Combustion

3.1 Definition

A premixed flame, where the reactants are completely mixed before combustion, is a self-sustaining propagation of a localized combustion zone, which can propagate at subsonic velocities or supersonic velocities (Turns, 2000). The premixed gases are broadly categorized into three types based on the speed and existence of the combustion wave in reacting mixtures (Kuo, 2005):

- **Explosion**
  Rate of heat generation is extremely fast, but it does not require the passage of a combustion wave through the exploding medium.

- **Deflagration**
  A combustion wave is propagating at a subsonic speed.

- **Detonation**
  A combustion wave is propagating at supersonic speed.

A deflagration wave is sustained by the chemical reaction, and its traveling speed is controlled by the heat conduction and radical diffusion (Glassman, 1996). However, in case of detonation, combustion is initiated through an advancement of a shock wave, which compresses and heats up the reactant mixture rapidly. Additionally, this shock wave, in turn, is sustained by the energy released from the combustion. The essential difference between a detonation and a deflagration wave is the pressure jump across the flame. One more substantial difference between these two are that the pressure increases greatly (the pressure in burnt side is generally 13-55 times higher than that in unburnt side: compression) across a detonation wave, while in deflagration, the pressure almost remains constant across the flame (actually there is a very small decrease: slight
expansion) (Kuo, 2005). Here, we mostly deal with the deflagration combustion wave, so called premixed flame.

3.2 Characteristics of Premixed Flame

Temperature profile of a flame is perhaps the best characteristics feature to worth looking at for complete understanding. Figure 3.1 shows a temperature profile in conjunction with other essential features of a typical premixed flame (Turns, 2000). A flame is a freely propagating wave when ignited in a chamber, full of unburnt reactants. The flame is always normal to the flame sheet. Continuity between burned and unburned mixtures gives:

\[ \rho_u S_L A \equiv \rho_u v_u A = \rho_b v_b A \]  

(3.1)

where \( S_L \) is flame speed, \( A \) is flame front area, and the subscripts \( u \) and \( b \) refer to the unburned and burned gases, respectively. Both the flame thickness and flame speed are thermo-chemical property (Peters, 2000), which primarily depend on the equivalence ratio, the temperature and pressure.

![Diagram](image_url)

Figure 3.1: Concentration and temperature profile of a stationary laminar, stoichiometric methane-air flame

When the flame is stretched (curved or strained or both), the flame speed is different from
the planar unstretched flame speed and very difficult to evaluate both by experimentally and numerically (Poinset & Veynante, 2001). The studies by several researcher suggest that the stretch \( \kappa \) is the only controlling parameter for flame structure in strain and curvature limits and there exist a linear relationship between stretched and unstretched flame speed based on asymptotic analysis (Poinset & Veynante, 2001). The expression for displacement and consumption speeds for stretched flame is given by

\[
\frac{s_d(0)}{s^0_L} = 1 - \frac{L^d_a}{s^0_L} \kappa \quad \text{and} \quad \frac{s_c}{s^0_L} = 1 - \frac{L^c_a}{s^0_L} \kappa
\]  

(3.2)

where \( s_d(0) \), \( s_c \), \( s^0_L \) are the displacement speeds, consumption speeds, unstretched flame speeds, and \( L^d_a \) & \( L^c_a \) are Markstein lengths. The displacement speed is defined on the fresh gas side. Two Markstein lengths are different and make the displacement and consumption speeds to behave differently to stretch, rewritten as

\[
\frac{s_d(0)}{s^0_L} = 1 - M^d_a \frac{\kappa \delta}{s^0_L} \quad \text{and} \quad \frac{s_c}{s^0_L} = 1 - M^c_a \frac{\kappa \delta}{s^0_L}
\]  

(3.3)

where \( \delta \) is unstretched flame thickness defined as

\[
\delta = \frac{\lambda_1}{\rho_1 C_v s^0_L} = \frac{D_{th}^1}{s^0_L} = \frac{\text{thermal diffusivity in fresh gas}}{\text{unstretched flame speeds}}
\]  

(3.4)

and \( M^d_a = L^d_a / \delta \) and \( M^c_a = L^c_a / \delta \) are Markstein numbers for the displacement and the consumption speeds, respectively. The expression \( \kappa \delta / s^0_L \) is a reduced Karlovitz number. There are various expressions for Markstein numbers proposed by several researchers and available. Clavin and Joulin (1983) proposed an expression for Markstein lengths as

\[
M^d_a = \frac{1}{\beta} \ln \frac{1}{1 - \beta} + \frac{Ze(Le - 1)(1 - \beta)}{2\beta} \int_0^\beta \frac{\ln(1 + x)}{x} dx
\]  

(3.5)

\[
M^c_a = \frac{Ze(Le - 1)(1 - \beta)}{2\beta} \int_0^\beta \frac{\ln(1 + x)}{x} dx
\]  

(3.6)

where \( Ze = E(T_b - T_a) / RT_b^2 \) is the Zeldovich number, \( Le \) is Lewis number of the deficient reactant, \( R \) is the universal gas constant, \( E \) is the activation energy. \( \beta \) is a nondimensional
temperature, defined as

$$\beta = \frac{(T_b - T_u)}{T_b}$$

(3.7)

here $T_b$ and $T_u$ are temperatures for burned and unburned gases, respectively. Lewis number is an important parameter, which is a ratio of thermal diffusivity and mass diffusivity, defined as

$$Le = \frac{D_{th}}{D} = \frac{\text{thermal diffusivity}}{\text{mass diffusivity}} = \frac{Sc}{Pr} = \frac{\text{Schmidt number}}{\text{Prandtl number}}$$

(3.8)

Equations (3.5, 3.6) shows that if Lewis number becomes less than unity, then Markstein lengths may become negative. The flame speed of a wrinkled flame front with positive curvature (the flame front is convex with respect to the unburnt side) becomes higher that $s_L^0$ due to negative Markstein lengths and vice versa. Due to this, the flame wrinkling is automatically increased, and the flame surface as well. Since, the Lewis number of a hydrogen-air mixture is less than unity, that explains the explosion of that mixture. This phenomenon is referred as a diffusion-thermal instabilities (Sivashinsky, 1977; Williams, 1985b).

Mostly the flame contains two zones: one is preheat zone and the other one is reaction zone. In preheat zone, the initial heat is released whereas in reaction zone bulk of the chemical energy is released. Usually, flame thickness is quite thin at atmospheric pressure and the chemical reaction takes place fastly at the initial stage and then slows down, by that time temperature gradient shoots up & leads to the formation of burned products. Normally, the burned gases are produced through the reaction of radicals (H, OH, O, and so on) of reactant mixtures, which are highly reactive atoms or atoms clusters that have unpaired electrons (Turns, 2000). The reaction of these radicals takes place through a sequence of chain reactions: first of all one molecule dissociates to form some radical species, and then this radical reacts to produce another radical species in a chain mechanism. The chain reaction usually fall into some categories based on the number of consumed radicals and produced radicals, such as: chain-initiation, chain-propagating, chain-termination and chain-branching reactions (Glassman, 1996; Turns, 2000).
The stable species are formed through the chain-termination reaction, where two radicals react to form a stable products and break the chain. At lower temperature, this type of reactions often turn out to be faster than any other type of chain reactions (Glassman, 1996). A chain-termination reaction in hydrocarbon combustion usually looks like \( H + OH + M \rightarrow H_2O + M \). However, on the other hand, two radical species are formed \( (O + H_2O \rightarrow OH + OH) \) by consuming one radical in a chain-branching reaction, which effectively increases the concentration of radical species in a faster rate and hence expedites the product formation process. There always exist a critical temperature, known as crossover temperature, above which the effects of chain-branching reactions become predominant over chain-termination reactions, resulting a self-sustained propagating flame. For hydrocarbon flames the critical temperature is around 1300 K at ambient pressure (Peters, 2000). The temperature profiles, mass fraction of species and other important features of a premixed flame can be obtained using CFD tools through detailed or simplified chemical mechanism. Figure 3.1 shows a schematic illustration of the inner structure of a stationary, laminar stoichiometric methane-air flame.

3.3 **Regimes in Turbulent Premixed Combustion**

Turbulent flow field and reaction are mutually related with each other. Turbulence increases the consumption rates of the reactants, which automatically enhances the reaction rate (increase heat...
release) and vice versa. This is highly desired for design consideration of a combustion engine. Figure 3.2 shows a schematic drawing of an idealized steady premixed flame in a duct, where the unburnt mixture enters into the mean turbulent flame zone in a direction normal to the mean front at a speed much higher than the laminar flame speed \( S_L \), which is known as turbulent flame speed \( S_T \).

Damköhler (1940), who was the first one, presented the theoretical expressions for the turbulent burning velocity \( S_T \). He also identified two different regimes of turbulent premixed combustion: one is the small-intensity, large scale turbulence and other one is high intensity, small scale turbulence. Equating the mass flux through the cross sectional area \( A \), Damköhler proposed an expression for burning velocity ratio as

\[
\frac{S_T}{S_L} = \frac{A_L}{A}
\]  

(3.9)

where \( A_L \) is laminar lame front area and \( A \) is the mean turbulent flame area. For small intensity, large scale turbulence, Damköhler’s assumption was that the interaction between wrinkled flame front and the turbulent flow field is purely kinematic. From geometrical analogy of Bunsen flame, he proposed a relation between wrinkled surface area and velocity fluctuation as

\[
\frac{A_L}{A} \sim \frac{v'}{S_L}
\]  

(3.10)

which in the limit of large \( v'/S_L \) is nothing but a kinematic scaling. For high intensity, small scale turbulence, Damköhler’s argument was that the turbulence only modifies the transport between the reaction zone and unburned gas, hence came up with a scaling analogy for laminar burning velocity as

\[
S_L \sim \left( \frac{D}{t_c} \right)^{1/2}
\]  

(3.11)

where \( D \) is the molecular diffusivity and \( t_c \) is the chemical time scale. Turbulent burning velocity is estimated in similar fashion as

\[
S_T \sim \left( \frac{Dt}{t_c} \right)^{1/2}
\]  

(3.12)
where $D_t$ is turbulent diffusivity. Combining equation 3.11 and 3.12, the velocity ratio is found as

$$\frac{S_T}{S_L} \sim \left( \frac{D_t}{D} \right)^{1/2}$$

Peters (2000) identified the corrugated flamelets regime with large scale turbulence and thin reaction zone regime with small scale as shown in Figure 3.3. For large scale turbulence the Kolmogorov scale is larger than the flame thickness, and the turbulence wrinkles the flame without disturbing its local structure. For small scale turbulence, the Kolmogorov scale is smaller than the preheat zone; as a result of that, it enters into the preheat zone, and enhances the transport of radicals and heat between the reaction zone and the unburned gas. Several researcher conducted a large number of experiments for measuring the turbulent flame speed with different combustion configurations, such as counter-flow flame, Bunsen flame, swirling flame and so on. Bradley (1992) published an extensive review article on the turbulent flame speed. It is well known that the turbulent flame speed increases almost linearly with the turbulence level at low turbulence intensity. Moreover, quenching of turbulent flame occurs, if the turbulence levels are higher than
some critical value, and the turbulent flame speed increase slightly. The quenching effect is also regarded as turbulent flame speed bending in combustion literature (Bradley, 1992). Turbulent combustion diagram is classified into different regimes for better understanding of influence of different turbulence level on turbulent combustion (Figure 3.3). In order to do this, a few nondimensional parameters are introduced and discussed.

For the shake of scaling purposes, it is helpful to assume equal diffusivities for all reactive scalars, and Schmidt number, Lewis number and Prandtl number to unity, defined as

\[
Le = \frac{D_{th}}{D} = 1; \quad Pr = \frac{\nu}{D_{th}} = 1; \quad Sc = \frac{\nu}{D} = 1
\]

(3.13)

where \( \nu, D_{th}, \) and \( D \) are the momentum, thermal and mass diffusivity, respectively. The laminar flame thickness \( l_F \) and the flame time \( t_F \) are given as

\[
l_F = \frac{D}{S_L}; \quad t_F = \frac{D}{S_L^2}
\]

(3.14)

The turbulent Reynolds number \( Re_t \) is expressed in terms of turbulent intensity \( \nu' \) and turbulent length scale \( l \) as

\[
Re_t = \frac{\nu'l}{S_L l_F}
\]

(3.15)

The turbulent Damköhler number \( Da \) is defined as the ratio of turbulent integral time scale to chemical time scale

\[
Da = \frac{\text{turbulent time scale}}{\text{chemical time scale}} = \frac{S_L l}{\nu'l_F}
\]

(3.16)

The Karlovitz number is the ratio of chemical time scale to Kolmogorov time scale, is given as

\[
Ka = \frac{\text{chemical time scale}}{\text{Kolmogorov time scale}} = \frac{l^2_F}{\eta^2}
\]

(3.17)

Using the above mentioned definitions (3.15, 3.16 and 3.17), a new relationship can be established as

\[
Re_t = Da^2 Ka^2
\]

(3.18)

Figure 3.3 shows the turbulent premixed combustion diagram in terms of length and velocity scales in log-log scale. The whole diagram is categorized into five different regimes.
The lower-left corner of the Figure 3.3, which is defined as laminar flame regimes, is separated from all turbulent flame regimes by the line Re$_t$=1. The wrinkled flamelets regime is not of much practical interest, because the fluctuation velocity $v'$ is less than the laminar flame speed in this regime. The line with $K\alpha$=1 is called the Klimov-Williams criterion, which means the flame thickness is equal to Kolmogorov length scale. Below this line, the flame thickness is thinner than the Kolmogorov length scale, and the regime ($K\alpha<1$ and $v'/S_L>1$) is called the corrugated flamelets regime, in which the flame front usually remains quasi-laminar.

The thin reaction zones regime is characterized by Re$_t$>1, $K\alpha_{\delta}<1$, and $K\alpha>1$, in which smallest eddies of size $\eta$ can enter into the reactive-diffusive flame structure since $\eta<l_F$. The $K\alpha_{\delta}=1$ corresponds to the situation that the Kolmogorov length scale is equal to the inner layer thickness, that assumes the inner layer thickness is one tenth of the flame thickness $l_F$, hence $\delta=0.1$ to $K\alpha=100$. Peters (2000) gave an argument that in this regime, the Kolmogorov eddies of size $\eta$ can enter into preheat zone but can not penetrate into the inner layer, a $l_{\delta}<\eta<l_F$, where $l_{\delta}$ is the thickness of the inner layer. Due to this, this regime is also known as thickened wrinkled flame (Poinso & Veynante, 2001). The regime above the line $K\alpha_{\delta}>1$ is called broken reaction zones, where the thin flame is no longer identified because both the preheat zone and the inner layer are disturbed by the turbulent eddies.

The line corresponding to Da=1 is very significant, because above this limit the turbulence time scale become shorter than chemical time scale, hence whole reaction is controlled by chemistry. This zones is often known as well-stirred reactor. Although, this particular regime is very difficult to access in practical combustion systems, since complete fast mixing without quenching is almost impossible to achieve (Glassman, 1996). However, in theoretical analysis, it is useful to have an estimation of maximum overall energy release in a specified volume.

3.4 Turbulent Premixed Combustion: Numerical Modeling

Practically, turbulent flows are numerically simulated using averaged or filtered governing
equations, in which those unclosed terms are modeled with the resolved variables. However, the nonlinearity of the averaged or filtered Arrhenius based reaction rate expressions, based on resolved variables (e.g. mean temperature, species mass fractions), makes it difficult to evaluate. Nevertheless, the mean reaction rates are often modeled from physical analysis. There are plenty of reviews available in literature regarding combustion models (Bray, 1996; Brewster et al., 1999; Candel et al., 1999; Veynante & Vervisch, 2002), so far lots of different turbulent combustion models have been developed and developing though. Few of the methodologies of turbulent premixed combustion modeling have been discussed here. Mostly, the concepts of RANS combustion models are extended to LES framework with certain modification, since RANS combustion models were developed much earlier than that of LES, and are in more matured state than LES combustion models. The following section usually deals with models in RANS framework, unless or otherwise explicitly mentioned.

3.4.1 Eddy-break-up Model

This model was first proposed by Spalding (1971). The idea behind that is chemistry does not play a major role while turbulent motion controls the reaction rate ($Re >> 1$ and $Da >> 1$). The reaction zone is viewed as a collection of fresh and burned gaseous pockets transported by turbulent eddies (Peters, 2000). The mean reaction rate for the product is given as

$$\overline{\omega_p} = C_{EBU} \rho \left( \overline{Y_p^{*2}} \right)^{1/2} / t_{EBU}$$

(3.19)

where $\overline{Y_p^{*2}}$ is the variation of mass fraction of product. The turbulent mixing time $t_{EBU}$ is calculated from turbulent kinetic energy $\kappa$ and its dissipation rate $\varepsilon$, as

$$t_{EBU} = \frac{\kappa}{\varepsilon}$$

(3.20)

Here $\overline{Y_p^{*2}}$ needs to be modeled properly. Magnussen and Hjertager (1977) proposed eddy-dissipation-concept (EDC) model based on similar type of argument.
The expression of reaction rate term, which is very simple function of known mean quantities, makes this model attractive. However, the obvious limitation is that it does not include any effects of chemical kinetics. The constants \(C_{EBU} \) needs fine tuning according to the problems and the model sometimes tries to overestimate the reaction rate, especially in highly strained regions. Nevertheless, the simplicity made this model to be used in many commercial CFD packages.

### 3.4.2 Bray-Moss-Libby model

Bray et al. (1977) proposed this model, which is based on the classical flamelet concept (flame front is infinitely thin) for premixed turbulent combustion. It may be considered as presumed pdf model, because it introduces the progress variable \( c \), a scalar quantity, is assumed to be bimodal: unburnt \((c = 0)\) or burnt \((c = 1)\). The progress variable \( c \) can be a normalized temperature or normalized product mass fraction.

\[
c = \frac{T - T_u}{T_b - T_u} \quad \text{or} \quad c = \frac{Y_p}{Y_{p,b}}
\]

The BML model has some important characteristics of turbulent premixed combustion like counter-gradient turbulent transport and flame induced turbulence generation (Poinsot & Veynante, 2001). The pdf of the progress variable \( c \) at any given location is expressed in terms of two Dirac delta function as

\[
P(c, x, t) = \alpha(x, t)\delta(x, c) + \beta(x, t)\delta(1 - c)
\]

where \( \alpha \) and \( \beta \) are the probabilities to find unburnt and burnt mixtures at location \( x \) and time \( t \).

The normalization condition yields

\[
\alpha(x, t) + \beta(x, t) = 1
\]

The pdf assumption in 3.22 provides an important assumption is that either the combustion system is in equilibrium (chemically) or in unburnt state due to improbable existence of intermediate states. Few more relations can be obtained from the definition as

\[
\bar{\rho c} = \int_0^1 \rho c^* P(c^*) dc^* = \rho_b \beta
\]
\[ \bar{p} = \int_0^1 \rho P(c^*) dc^* = \alpha \bar{\rho}_u + \rho_b \beta \quad (3.25) \]

where subscripts \( u \) and \( b \) designate the unburnt and burnt side respectively. Any Favre quantity \( \phi \) can be defined as

\[ \tilde{\phi} = (1 - \bar{c})\tilde{\phi}_u + \bar{c}\tilde{\phi}_b \quad (3.26) \]

Here, \( \tilde{\phi}_u \) and \( \tilde{\phi}_b \) are the conditional average of \( \phi \) for any given \( c \) value between 0 and 1. Therefore, the scalar turbulent flux \( \bar{\rho}u^\prime c^\prime \) can be expressed as:

\[ \bar{\rho}u^\prime c^\prime = \bar{\rho} (\bar{u}c - \bar{u}c) = \bar{\rho} (\bar{c} \bar{u}_b - \bar{u}c) = \bar{\rho} \bar{c} (1 - \bar{c})(\bar{u}_b - \bar{u}_u) \quad (3.27) \]

For steady one dimensional flame, the mean velocity increases towards burned side, but the mass flow rate remains constant as the density decreases. Hence, it is expected that the difference of the local conditional velocities \( (\bar{u}_b - \bar{u}_u) \) is always greater than zero, and therefore \( u^\prime c^\prime > 0 \). This conflicts with the gradient transport assumption

\[ -u^\prime c^\prime = D_t \frac{\partial \bar{c}}{\partial x} \quad (3.28) \]

which needs \( u^\prime c^\prime < 0 \) since \( \partial \bar{c}/\partial x > 0 \). This phenomenon is known as countergradient diffusion (Bray et al., 1981). DNS (Wenzel & Peters, 2000) showed that turbulent mixing plays the main role in gradient diffusion, while the gas expansion effect in countergradient diffusion. The modeling of chemical source term in BML mode is usually done in three main approaches: one is based on scalar dissipation rate, one is on flame crossing frequency and one is on flame surface density (Poinset & Veynante, 2001).

### 3.4.3 Statistical Approach: Probability Density Function Model

The probability density function (pdf) is a stochastic method, which directly considers the probability distribution of the relevant stochastic quantities in a turbulent reacting flow. In turbulent flows, the pdf \( P \) is a function of both the position in space \( x \) and the time \( t \). Then, \( P(U; x, t)dU \) denotes the probability of finding a value \( u \) within the range \( u \in U - dU/2, U + dU/2 \) at the
position $x$ and time $t$. If $P$ is known, the mean value of a quantity is defined as the first moment as:

$$\bar{u} = \int_{-\infty}^{+\infty} u P(u; x, t) du$$

(3.29)

and the variance of $u$ is defined by the second central moment,

$$\overline{u^2} = \int_{-\infty}^{+\infty} (u - \bar{u})^2 P(u; x, t) du$$

(3.30)

This idea can easily be extended to take into account multiple variables. For example, the instantaneous reaction rate is a function of species mass fractions and temperature as

$$\omega = \omega(Y_1, Y_2, ..., T)$$

(3.31)

and if the joint probability $P(Y_1, Y_2, ..., T)$ for $Y_1, Y_2, ..., T$ in the range

$$Y_1 \in Y_1 - dY_1 / 2, Y_1 + dY_1 / 2$$

$$Y_2 \in Y_2 - dY_2 / 2, Y_2 + dY_2 / 2$$

................

$$T \in T - dT / 2, T + dT / 2$$

is known, then the mean reaction rate $\overline{\omega}$ is determined as

$$\overline{\omega} = \int_{y_1, y_2, ..., T} \omega(Y_1, Y_2, ..., T) P(Y_1, Y_2, ..., T) dY_1, dY_2, ..., dT$$

(3.33)

This kind of pdf description of turbulent reacting flow has some theoretical benefits, such as the complex chemistry is taken care of without applying any ad-hoc assumptions (like ‘flamelet’ or ‘fast reaction’). Moreover, it can be applied to non-premixed, premixed, and partially premixed flames without having much difficulties. Usually, there are two ways which are mainly used to calculate the pdf

(a) presumed pdf approach

(b) pdf transport balance equation approach

3.4.3.1 Presumed Pdf Approach

The main philosophy behind presumed pdf method is to ‘presume the shape of the pdf $P’. 

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Usually, a pdf function can take any shape and have multiple extrema. It not only contains the information on mean value, but also on its variance, and all higher moments. Since, pdf functions show some common features in many different combustion applications, it is reasonable enough to represent them with a special shape but with different controlling parameters. The most popular approach is to assume the pdf function as a $\beta$ function, and its controlling parameters are the mean and variance of the variable (Borghi, 1988). It has the form as:

$$P(f) = \frac{f^{a-1}(1 - f)^{b-1}}{\int_0^1 f^{a-1}(1 - f)^{b-1}df}$$  \hspace{1cm} (3.34)

$$a = \tilde{f} \left[ \frac{\tilde{f}(1 - \tilde{f})}{\tilde{f}^{n/2}} - 1 \right], \quad b = \frac{a}{\tilde{f}} - a$$  \hspace{1cm} (3.35)

The main disadvantage of this presumed pdf method is that it is not so easy to guess or measure joint pdf of multiple variables (Pope, 1985). More simple approach is to presume that these variables are statistical independent. Thus, a joint pdf function, e.g. $P(\phi, \varphi, \gamma)$, can be defined as

$$P(\phi, \varphi, \gamma) = P_\phi(\phi)P_\varphi(\varphi)P_\gamma(\gamma)$$  \hspace{1cm} (3.36)

Unfortunately, this assumption does not hold good for practical combustion applications, since temperature, species mass fraction are closely related in flames (Poinsot & Veynante, 2001).

### 3.4.3.2 Pdf Transport Balance Equation

A transport equation for pdf function is solved in this approach. This balance equation can be written for multi species, mass-weighted probability density function. There are several different ways for derivation of this transport equation (Pope, 1985; Vervisch et al., 1995). For multi species, density-weighted joint pdf, $P(f_1, f_2, \ldots, f_n)$, the transport equation is expressed as (Pope,
(3.37):
\[
\bar{\rho} \frac{\partial \bar{P}}{\partial t} + \bar{\rho} \bar{u}_i \frac{\partial \bar{P}}{\partial x_i} = - \frac{\partial}{\partial x_i} \left[ \bar{\rho} \left( \frac{u_i}{Y = f} \right) \bar{P} \right] \\
\text{Turbulent convection}
\]
\[
-\bar{\rho} \sum_{j=1}^{n} \sum_{k=1}^{n} \frac{\partial}{\partial f_j} \frac{\partial}{\partial f_k} \left[ D \left( \frac{\partial Y_j}{\partial x_i} \frac{\partial Y_k}{\partial x_i} | Y = f \right) \bar{P} \right] \\
\text{Molecular mixing}
\]
\[
-\bar{\rho} \sum_{j=1}^{n} \frac{\partial}{\partial f_j} \left[ \omega \left( f_1, f_2, f_3, ..., f_n \right) \bar{P} \right] \\
\text{Chemical reaction}
\]

Here the operator \( \bar{Q} \left| Y = f \right. \) corresponds to the conditional averaging of variable \( Q \) for the sampling variable \( f_j \). The chemical reaction term in 3.37 is in closed form and hence does not require any modeling and can handle any complex reaction mechanism without having much difficulties. On this regard, it is often claimed that the transport pdf method has considerable advantage over any other turbulent combustion models (Peters, 2000).

The first three terms in equation 3.37 are unsteady evolution, convection of flow field and turbulent convection, respectively. These three terms describe the pdf evolution in physical space. However, the molecular mixing and chemical reaction describe the pdf evolution in the composition space \((f_i) \). Since this approach is based on local one-point statistical approach, it is difficult to model the unclosed molecular mixing terms in 3.37, however, the spatial gradient in the unclosed term requires additional spatial information (Poinsot & Veynante, 2001). One more major drawback of transport pdf approach is its high dimensionality, which essentially makes the implementation of this approach to different numerical techniques, like FVM or FEM, limited, since their memory requirements increase almost exponentially with dimensionality. Usually, Monte-Carlo algorithms, which reduce the memory requirements, are used (Pope, 1985). However, a large number of particles need to be present in each grid cell to reduce the statistical
error, essentially that makes it a very time consuming process. So far, the transport equation method is only applied to relatively simple situations (Poinsot & Veynante, 2001).

Jones and Prasetyo (1996) carried out a calculation for a premixed turbulent counter flow jet configuration using a five-scalar joint pdf transport equation. They used two different models for closing the unknown molecular mixing term in 3.37 and presented a comparative study. A four step reduced mechanism by Jones and Lindstedt (1988) was used. The flow equations in conjunction with $\kappa - \varepsilon$ turbulence model was solved using standard finite difference methods, whereas the pdf transport equation was solved using a Monte-Carlo technique. Apart from carbon monoxide prediction, the computed data is in good agreement with measured data set.

3.4.4 Flamelet Theory

The concept of flamelet was proposed by Williams (1975). According to his definition, turbulent flame can be viewed as an ensemble of locally stretched laminar flames, so called flamelets. Flamelets are thin reactive-diffusive layers, which are embedded in an otherwise no reacting turbulent flow field. The interaction between turbulence and chemistry are taken place through this mechanism: the flamelet leases heat to the flow field, hence the flow accelerates across the flame front and changes the turbulent flow fields on both side of flame front; on the other hand, the turbulent eddies convect and distort the flame front without disturbing the structure of flamelets. This mechanism helps to decouple the calculation of turbulence and chemistry and provides an added advantage for turbulent combustion modeling.

The idea of flamelet concept is completely based on the assumption that turbulence can not disturb the structure of flamelets. Qualitative kinetic analysis shows that the Kolmogorov length scale must be larger than the flame thickness, i.e. the Karlovitz number is less than one, to support the idea of flamelet. Corrugated flamelets and wrinkled flamelets regimes (Figure 3.3), which are separated from other regimes with the line $Ka=1$ (Klimov-Williams criterion), are suitable for flamelet concept. However, experimental and numerical studies by several researcher (Poinsot et
al., 1991; Shepherd et al., 2002; Baum et al., 1994; Buschmann et al., 1996; Sankaran & Menon, 2000) showed that this regime may be extended to large Karlovitz number. Moreover for large $Ka(Ka >> 1)$, the turbulent eddies increase the heat and species diffusion due to broadening of preheat zone, but the reaction zone still remains thin near the flame front as the eddies do not penetrate the thin reaction zone because of the increased viscous dissipation by high temperature. The effect of increased turbulence is usually manifested as wrinkled flame front, which contrarily increase the reaction rate without affecting the thin layer structure. Therefore, Peters (1999 & 2000) proposed that the flamelet concept is suitable for the region upto $Ka < 100$ as shown in Figure 3.3.

The laminar flame structure has great importance in use of flamelet concept. The article by Williams (2000) shows the detailed numerical study of flamelet structures for premixed, diffusion and partially premixed flames. A detailed description of flamelet equations derivation is found in Peters (2000) and the references therein. Mostly in flamelet approaches, the location of the flamelet in a turbulent flow field is usually defined by a geometrical surface: iso-$Z$ (mixture fraction) surface for diffusion flames, iso-$c$ (progress variable) or iso-$G$ (signed distance function) surfaces for premixed flames. However in partially premixed combustion, combined flamelet models, like a flamelet model for diffusion flame and a flamelet model for premixed flame, are generally solved together as in Chen et al., (2000), where a $Z$-equation and a $G$-equation are solved simultaneously.

3.4.5 Models Based on Geometrical Description

Generally, the flame is described as a geometrical surface in the geometrical analysis and this approach can easily be linked to the flamelet theory (the flame is thin compared to all flow scales). With this idea, scalar fields ($c$ or $Z$) are studied in terms of dynamics and physical properties of iso-value surface denoted as flame surfaces (iso-$c$ or iso-$Z$). The flame is then viewed just as an interface between fuel and oxidizer (diffusion type flame) or between fresh and burnt gases
(premixed type flames). This leads to the flamelet modeling based on geometrical analysis, and few of them are discussed briefly here.

3.4.5.1 \( c \)-equation Model

The progress variable for an adiabatic premixed combustion with one-step, irreversible chemistry (assuming constant specific heat capacity for all reacting species) is defines as

\[ c = \frac{T - T_u}{T_b - T_u} \]

The balance equation (Boger et al. 1998) for \( c \) be written as:

\[ \frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho uc) = \nabla \cdot (\rho D \nabla c) + \dot{\omega}_c \]  \hspace{1cm} (3.38)

\[ \frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho uc) = \rho s_d |\nabla c| \]  \hspace{1cm} (3.39)

where \( D \) is the molecular diffusivity, \( u \) is velocity vector. Equation 3.39 is another form of \( c \) equation which is written in terms of front displacement speed \( s_d \). After applying the filtering operation, the LES filtered equations become

\[ \frac{\partial \bar{\rho} \bar{c}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{c}) = \nabla \cdot (\bar{\rho} D \nabla \bar{c}) + \bar{\omega}_c - \nabla \cdot [\bar{\rho} (\bar{u} \bar{c} - \bar{u} \bar{c})] \]  \hspace{1cm} (3.40)

\[ \frac{\partial \bar{\rho} \bar{c}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{c}) = \bar{s}_d |\nabla \bar{c}| - \nabla \cdot [\bar{\rho} (\bar{u} \bar{c} - \bar{u} \bar{c})] \]  \hspace{1cm} (3.41)

The terms on the l.h.s. of the equations respectively are unsteady terms and convective fluxes, whereas the r.h.s terms in equation 3.40 are filtered molecular diffusion, filtered reaction rate and unresolved convective flux respectively. The unresolved convective flux is modeled using gradient diffusion hypothesis as

\[ \bar{\rho} (\bar{u} \bar{c} - \bar{u} \bar{c}) = -\frac{\mu_t}{Sc_t} \nabla \bar{c} \]  \hspace{1cm} (3.42)

However, several researcher proposed different methods for modeling the term \( \bar{s}_d |\nabla \bar{c}| \) in equation 3.41, few of them are briefly discussed in the following sections.
3.4.5.2 Flame Surface Density Model

The flame is identified as a surface and the flame surface density $\Sigma$ is introduced to define the unclosed term in 3.41. $\Sigma$ measures the available flame area $\delta A$ per unit volume $\delta V$ (unit: m$^2$/m$^3$). In order to calculate $\Sigma$, both algebraic expressions (Boger et al. 1998) and transport equations (Boger et al. 1998; Hawkes & Cant, 2000 and 2001) have been developed. The algebraic relation is expressed as:

$$\rho s_d |\nabla c| = \rho_u S_L \Sigma$$

(3.43)

The transport equation by Hawkes and Cant (2001) is expressed as:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial (\tilde{u}_i \Sigma)}{\partial x_i} + \frac{\partial}{\partial x_i} \left( (\overline{u_i}_s - \tilde{u}_i) \Sigma \right) = \frac{(\alpha_T)_s \Sigma - \frac{\partial}{\partial x_i} \left( (S_L N_i)_s \Sigma \right)}{S_L \frac{\partial N_i}{\partial x_i}} \Sigma$$

(3.44)

where the subscript $s$ represents the subgrid scale. The three terms on the l.h.s of equation 3.44 are rate of change, mean convection and subgrid convection respectively, and the r.h.s terms are defined as effect of fluid strain, propagation term and the production of flame surface density subjected to curvature and propagation effect, respectively. Boger et al. (1998) proposed that the last four terms in equation 3.44 are unclosed and can be easily estimated from DNS or experimental data, since they are physically well defined terms.

3.4.5.3 Flame Wrinkling Model

The idea of this model came from flame surface density model. The basic concept is to introduce the ratio $\Xi$ of the turbulent flame surface to its projection in the flame propagation direction. Weller (1993) proposed a detailed derivation of this model in RANS framework. However, Weller et al. (1998) proposed a new flame wrinkling model in LES framework and thereafter Fureby (2000) applied the same to study the combustion instabilities in jet engine afterburner. The model considers a regress variable $b$, which represents the unburnt gas mass fraction and is related with $c$ as $b = 1 - c$. The transport equation is obtained after filtering the
conditional transport equation of $b$ as:
\[
\frac{\partial \rho_b \tilde{\Phi}}{\partial t} + \nabla \cdot \left( \rho_b \tilde{\Phi} \right) = \nabla \cdot (\rho D \nabla \hat{b}) - \rho_a S_L \Xi \left| \nabla \hat{b} \right|
\]

and the transport equation for flame wrinkle density $\Xi$ is defined as:
\[
\frac{\partial \Xi}{\partial t} + \hat{u}_s \nabla \Xi = G \Xi - R(\Xi - 1) + (\sigma_s - \sigma_t) \Xi
\]

where $\hat{u}_s$ is the surface filtered effective velocity of the flame, $G \Xi$ and $R(\Xi - 1)$ are the subgrid turbulent generation and removal rates, respectively. These three terms are proposed by Weller et al. (1998). However, $\sigma_s$ and $\sigma_t$ are resolved strain rates and defined using resolved quantities. Additionally, Weller et al. (1998) also proposed a transport equation for laminar flame speed $S_L$ to account the strain rate influence on laminar flame speed. The transport equation for laminar flame speed is expressed as
\[
\frac{\partial S_L}{\partial t} + \hat{u}_s \nabla S_L = -\sigma_s S_L + \sigma_s S_L^\infty \left( \frac{S_L^0 - S_L}{S_L^\infty - S_L^0} \right)
\]

(3.45)

the detailed information regarding the terms in equation 3.45 are found in Weller et al. (1998). Moreover, Knikker et al. (2000) reported the validation studies on flame surface density $\Sigma$ and flame wrinkling density $\Xi$ on LES framework.

3.4.5.4 Turbulent Flame Closure Model

The so called turbulent flame closer model (TFC) essentially estimates the unclosed term in 3.41 based the turbulent flame speed. The unclosed term in this approach is defined as
\[
\overline{\rho_s d | \nabla c |} = \rho_a u_{sg} | \nabla c |
\]

(3.46)

where $u_{sg}$ is the subgrid turbulent speed in LES framework. Zimont (1979) first proposed the TFC model, and recently Karpov et al. (1996), Zimont (2000) applied on some premixed combustion calculation. Zimont (2000) proposed an expression for the turbulent flame speed $S_T$ in RANS framework based on the Kolmogorov assumption of the equilibrium fine-scale turbulence and the assumption of the universal small-scale structure of the wrinkled flamelet sheet. It is defined as
\[
S_T = Cu' (Da)^{1/4}
\]

(3.47)
where $C$ is a constant parameter, having value around 0.5 and $Da$ is the Damköhler number.

In LES framework the TFC model was applied by Flohr and Pitsch (2000), Zimont and Battaglia (2003). Flohr and Pitsch (2000) proposed an expression for subgrid turbulent speed as

$$u_{sg}/S_L = 1 + C \left( Re_\Delta Pr \right)^{1/2} Da^{-1/4}$$  \hspace{1cm} (3.48)

where $Re_\Delta = u_\Delta \Delta / \nu$. The subgrid turbulent velocity $u'_\Delta$ is estimated as

$$u'_\Delta = C_s \Delta \left( 2 \tilde{S}_{ij} \tilde{S}_{ij} \right)^{1/2}$$  \hspace{1cm} (3.49)

3.4.5.5 G-equation Model

In G-equation model, the flame front is described as a propagating surface, which is tracked using a field variable or iso-surface $G_0$. The filtered G-equation in LES framework expressed as

$$\frac{\partial \tilde{G}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{p} \tilde{u}_i \tilde{G} \right) = \tilde{p} S_T \left| \nabla \tilde{G} \right|$$  \hspace{1cm} (3.50)

where $S_T$ is estimated by an algebraic formulation

$$S_T / S_L \approx 1 + C (u'_{\Delta} / S_L)$$  \hspace{1cm} (3.51)

the constant $C$ is calculated through dynamic procedure and subgrid turbulent velocity is estimated as

$$u'_{\Delta} \approx \Delta \left( 2 \tilde{S}_{ij} \tilde{S}_{ij} \right)^{1/2}$$  \hspace{1cm} (3.52)

Later, Im et al. (1997) revised the model by introducing an additional diffusive term to the transport equation of $G$. Similar modeling approaches have been proposed by Kim et al. (1999), Kim and Menon (2000), and Shinjo et al. (2003). For example the model proposed by Kim et al. (1999) is expressed as

$$\frac{\partial \tilde{G}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{p} \tilde{u}_i \tilde{G} \right) = \frac{\partial}{\partial x_i} \left( \mu_t \frac{\partial \tilde{G}}{\partial x_i} \right) + \tilde{p} S_T \left| \nabla \tilde{G} \right|$$  \hspace{1cm} (3.53)

where $\mu_t$ and $S_{C_{ij}}$ are the subgrid viscosity and Schmidt number, respectively. The subgrid flux in this formulation is modeled using gradient diffusion concept. However, Peters (2000) and Oberlack et al. (2001) argued that this gradient-diffusion assumption can not be used here, since it would result in an elliptic equation for $\tilde{G}$ and contradict the parabolic character of the original
The $G$-equation proposed by Peters (1999), is valid in both corrugated flamelets regime and thin reaction zone regime. Through asymptotic analysis, he considered a propagation term $S_L \left| \nabla G \right|$ in corrugated flamelets regime and a curvature term $D_k \left| \nabla G \right|$ in thin reaction regime. Therefore, the equation proposed by him in RANS framework has the form

$$\frac{\partial \tilde{p} \tilde{G}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{p} \tilde{u}_i \tilde{G} \right) = \tilde{p} S_L \left| \nabla \tilde{G} \right| - \tilde{p} D_k \left| \nabla \tilde{G} \right|$$  \hspace{1cm} (3.54)

Later on, Pitsch and Duchamp (2002), Duchamp and Pitsch (2002) extended this RANS formulation to LES framework without any modification. Moreover, many researchers (Peters, 1999; Oberlack et al. 2001) pointed out that the time and special averaging to traditional $G$-equation in RANS or LES framework is not logically valid, since these two averaging techniques implicitly assume that the $G$ scalar has the definition in entire field or domain, which is not the fact in reality.

Peters (2000) used a different averaging procedure, based on probability density function to find the flame surface at a particular location, for derivation of averaged $G$-equation in RANS framework. Oberlack et al. (2001) proposed a averaging procedure of $G$-equation for premixed combustion to account for a generalized scaling symmetry, and derived a modeling equation for the averaged flame location. However, Pitsch (2002) proposed a filter kernel that takes information only from the instantaneous flame surface and derived a modeled equation in LES framework, which has the form as

$$\frac{\partial \tilde{p} \tilde{G}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{p} \tilde{u}_i \tilde{G} \right) = \rho_u S_{T,a} \left| \nabla \tilde{G} \right|$$  \hspace{1cm} (3.55)

$$\frac{\partial \tilde{p} \tilde{G}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{p} \tilde{u}_i \tilde{G} \right) = \rho_b S_{T,b} \left| \nabla \tilde{G} \right|$$  \hspace{1cm} (3.56)

The fact of matter is that $G$-equation is only valid on the instantaneous flame front. In addition to the filtered $G$-equation, another phenomenon must be addressed, that is the signed-distance
function. The level set $G$-equation is usually used together with the signed-distance function, which views the scalar $G$ surrounding the front as the signed distance to the front. The signed distance function is well defined in the whole field and the usual filtering procedure is applied on it. However, the filtered scalar $G$ does not satisfy the signed distance function anymore, since

$$
|\nabla G| = 1, \quad |\nabla \tilde{G}| = 1 \tag{3.57}
$$

$$
\tilde{G} \neq G, \quad |\nabla \tilde{G}| \neq |\nabla G|, \quad |\nabla \tilde{G}| \neq 1
$$

Nilsson & Bai (2003) also discussed the similar relations in RANS time averaging procedure. However, for simplicity, most of the previous works (Chen et al., 2000; Pitsch & Duchamp, 2002; Duchamp & Pitsch, 2000) assumed and used the filtered or averaged $\tilde{G}$ as the signed distance function, i.e.

$$
|\nabla \tilde{G}| = 1 \tag{3.58}
$$

3.5 Concept of Artificially Thickened Flame Model

In this approach, the flame front is artificially thickened to resolve on LES mesh, and thereafter the filtered governing equation for species transport is solved along with N-S equations. The artificially thickened flame model is used in this thesis work and the detailed description is given in the following Chapter.
Chapter 4 LES of Turbulent Premixed Combustion Based on Artificially Thickened Flame Model

4.1 Background

To this end, multiple studies have been concentrated on diffusion (non-premixed) flames, while premixed cases have not received much attention. Because of the fact that infinitely fast chemistry constitute a useful path for studying diffusion flames, whereas such assumption is not well suited theor premixed studies. Moreover, the flame-turbulence interaction modeling in premixed combustion systems requires to tack the flame front position, resulting problem which is much more difficult to handle than most diffusion flames. Naturally, the obvious attempt is to track the flame front by solving its inner structure, but this becomes impossible to do on a computational grid due to the thin flame thickness. This leads to two major approaches which have been developed and tested so far.

(1) By treating the flame surface as an infinitely thin propagating surface (flamelet), eventually brings the flame thickness to zero. This is idea behind G-equation model as discussed previous chapter.

(2) By thickening the flame front to resolve on computation grid while propagating at the same speed as the unthickened flame. This is the principle of thickened flame (TF) model (Colin et al., 2000; Poinsot and Veynante, 2001).

Butler and O’Rourke (1977) was first to propose the idea of capturing a propagating premixed flame on a coarser grid. The philosophy is that the flame is artificially thickened by keeping the speed same as of laminar flame speed $s^0_f$. The standard TF model developed by Colin et al. (2000) is discussed in details and used in this work. The balance equation of $i$th species mass fraction $Y_i$
in a one-dimension premixed flame of thermal thickness $\delta_L^0$ and speed $s_L^0$ is

$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial}{\partial x} (\rho u Y_i) = \frac{\partial}{\partial x} \left( \rho D_i \frac{\partial Y_i}{\partial x} \right) + \dot{\omega}_i$$

(4.1)

The simple theories of laminar premixed flame (Williams, 1985; Kuo, 1986) define the flame speed $s_L^0$ and flame thickness $\delta_L^0$ as

$$s_L^0 = \alpha \sqrt{DB}, \quad \delta_L^0 = \frac{D}{\alpha s_L^0}$$

(4.2)

where $D$ is the molecular diffusivity and $\bar{B}$ is the mean reaction rate. If the flame thickness $\delta_L^0$ is increased by a factor of F with a constant flame speed $s_L^0$, that is easily achieved by replacing the thermal and molecular diffusivities $D_{th}$ and $D$ by $FD_{th}$ and $FD$, and the reaction rate $\bar{B}$ by $\bar{B}/F$. When F is sufficiently large (typically from 5 to 30), the thickened flame front is resolved on LES mesh ($\Delta_x$), which is usually less than typical premixed flame thickness (around 0.1-1 mm). Modifying the equation 4.1 by $X = Fx$ and $t' = Ft$ to have the following

$$\frac{\partial \rho Y_i}{\partial t'} + \frac{\partial}{\partial X} (\rho u Y_i) = \frac{\partial}{\partial X} \left( \rho (D_i F) \frac{\partial Y_i}{\partial X} \right) + \frac{\dot{\omega}_i}{F}$$

(4.3)

which is having the similar form like equation 4.1. Therefore, for a steady propagating laminar flame ($\partial / \partial t = \partial / \partial t' = 0$ and $\rho u = \rho_0 s_L^0$, where $\rho_0$ is the fresh gases density), equation 4.1 & 4.3 have same solutions apart from the thickening factor F (for eq. 4.3).

- **Advantages of TF Model**

There are multiple reasons which make this TF model very attractive for premixed combustion simulations. The reasons are:

(i) TF model propagates laminar premixed front at laminar speed exactly like G-equation approach. However, this flame propagation is due to the combination of diffusive and reactive terms which can also act independently, so that quenching (near walls for example) or ignition can be simulated.

(ii) From the numerical point of view, the chemical reaction is described as in a Direct Numerical Simulations (DNS) on the LES computational grid. The actual flame is just replaced
by a thicker laminar flame without filtering. Therefore, this formulation could not require a sub
grid scale model.

(iii) As Arrhenius law is used for calculation of reaction rate, various phenomena are directly
taken into account without requiring ad-hoc sub models.

(iv) Theoretically, this approach could be extended to simulate complex chemistry by applying
the same concept for different species.

(v) Equations 4.1 & 4.3 show that the flame responses to unsteady phenomena \( t \) is replaced
by \( t' = Ft \) and to strain rates induced by velocity field are modified by thickening procedure.
This does not have too much importance in practice as the flame speed remains as laminar speed
\( s^0_L \), however may lead to some difficulties while dealing with highly turbulent flow or complex
chemistry.

Therefore, the idea is extended from one-dimension to a system of balance equations and
expressed as

\[
\frac{\partial \rho Y_i}{\partial t'} + \nabla \cdot (\rho u Y_i) = \nabla \cdot ((\rho D_i F) \nabla Y_i) + \frac{\omega_i}{F} \tag{4.4}
\]

4.2 Description of Artificially Thickened Flame Model on LES Framework

In LES framework, the spatial filtering on species transport equation gives a filtered equation
for species involved in the reacting system. The filtered equation looks as

\[
\frac{\partial \rho \tilde{Y}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \tilde{\rho} \tilde{u}_j \tilde{Y}_i \right) = \frac{\partial}{\partial x_j} \left( \tilde{\rho} D_i \frac{\partial \tilde{Y}_i}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left[ \tilde{\rho} \left( \tilde{u}_j \tilde{Y}_i - \tilde{u}_j \tilde{Y}_i \right) \right] + \frac{\tilde{\omega}_i}{F} \tag{4.5}
\]

where the terms on r.h.s are filtered molecular diffusion flux, unresolved transport, and filtered
reaction rate respectively. In general, the unresolved term is modeled as gradient diffusion
assumption, however, in TF model, the thickening procedure takes care of that term and the
modified filtered equation 4.5 becomes

\[
\frac{\partial \rho \tilde{Y}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \tilde{\rho} \tilde{u}_j \tilde{Y}_i \right) = \frac{\partial}{\partial x_j} \left( \tilde{\rho} F D_i \frac{\partial \tilde{Y}_i}{\partial x_j} \right) + \frac{\tilde{\omega}_i}{F} \tag{4.6}
\]

Though the filtered thickened equation looks promising, the thickening of the flame by a factor of
F modifies the interaction between turbulence and chemistry as the Damköhler number, Da, which is a ratio of turbulent (τₜ) and chemical (τₑ) time scales is decreased by a factor F and becomes Da/F.

\[
Da = \frac{\tau _t}{\tau _e} = \frac{l_t}{l_e} \frac{s_0}{u' \delta _L^0}
\]  

(4.7)

It implies that the flame response to the turbulent motions and the flame surface wrinkling are modified due to flame thickening. Poinset et al. (1991) showed that when the turbulent length to laminar length scale ratio (lₜ/δₗ₀) is decreased, the flame becomes more and more intensive to the turbulent motions. However, the ratio is decreased by a factor F due to thickening. Contrarily, the thickened flame is more sensitive to strain than the actual flame (Angelberger et al., 1998). Hence, the sub grid scale effects have been incorporated into the thickened flame model based on the following hypothesis (Colin et al., 2000):

(i) Eddies smaller than \(F\delta _L^0\) do not interact with the flame any more and their effects have to be incorporated in the modeling as a sub grid scale effect.

(ii) Eddies larger than \(F\delta _L^0\) interact with the flame front but their efficiency might be affected by the increased flame thickness.

Therefore the subgrid scale effect is parametrized using an efficiency function E derived from DNS results (Angelberger et al., 1998; Charlette et al., 2002; Colin et al., 2000) of flame vortex interaction. This efficiency function measures the subgrid scale wrinkling as a function of the local subgrid turbulent velocity \(u'_{\Delta e}\) and the filter width \(\Delta e\). Incorporating the efficiency function E, into equation 4.6, it becomes

\[
\frac{\partial p\tilde{Y}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( p\tilde{u}_j\tilde{Y}_i \right) = \frac{\partial}{\partial x_j} \left( pEFD_i^{-1} \frac{\partial \tilde{Y}_i}{\partial x_j} \right) + E\tilde{\omega}_i \frac{\omega_i}{F}
\]  

(4.8)

Where the diffusivity ED, before multiplication by F to thicken the flame front, may be decomposed as \(ED = D + (E - 1)D\) and corresponds to the sum of the molecular diffusivity, D, and a turbulent sub grid scale diffusivity, \((E - 1)D\), depending on turbulence and flame characteristics.
In fact, \((E \cdot 1)D\) could be viewed as a turbulent diffusivity used to close the unresolved scalar transport in filtered equation 4.5. In the modified equation 4.8, the turbulent flame propagates with a speed \(s_T = E s_0^0\), while keeping the flame thickness \(\delta_L^1 = F s_0^0\). In laminar region, \(E\) goes to unity, and the equation 4.8 propagates the front with laminar speed of \(s_0^0\).

The central ingredient of the TF model is the sub grid scale wrinkling function \(E\), which is defined by introducing a dimensionless wrinkling factor \(\Xi\). The factor \(\Xi\) is the ratio of flame surface to its projection in the direction of propagation. Usually, it is larger in laminar flame than that of thickened flame due to that fact that the laminar flame exhibits more small scale cusps, which increases the flame surface. Thus, the efficiency function, \(E\), happens to be a function of the local filter size \((\Delta_e)\), local subgrid scale turbulent velocity \((u'_e)\), laminar flame speed \((s_0^0)\), laminar and the flame thickness \((\delta_0^0, \delta_L^1)\). Depending on the definition and modeling approaches, the efficiency function can be evaluated by using one of the following methods.

### 4.2.1 Original TF Model

Colin et al. (2000) proposed this model. They defined the following expression for the wrinkling factor \(\Xi\), based on the previous work of Maneveau and Poinsot (1991).

\[
\Xi = 1 + \beta \frac{u'_e}{s_L} \Gamma \left( \frac{\Delta_e}{\delta_0^0}, \frac{u'_e}{s_0^0} \right)
\]  
\[
(4.9)
\]

where

\[
\beta = \frac{2 \ln 2}{3 c_{ms} \left( \text{Re}_{t}^{1/2} - 1 \right)} \quad \text{and} \quad c_{ms} = 0.28
\]
\[
(4.10)
\]

\(\text{Re}_t = u l / \nu\) is turbulent Reynolds number. The increase of flame wrinkling due to turbulent stretch is expressed by the term \(\beta u'_e / s_L^0 \Gamma\). The local filter size \((\Delta_e)\) is related with laminar flame thickness as \(\Delta_e = \delta_L^1 = F \delta_0^0\). The function \(\Gamma\) represents the integration of the effective strain rate induced by all scales affected by the artificial thickening, i.e. between the Kolmogorov \(\eta_k\) and the filter \(\Delta_e\) scales. \(\Gamma\) is defined as:

\[
\Gamma \left( \frac{\Delta_e}{\delta_0^0}, \frac{u'_e}{s_L^0} \right) = 0.75 \exp \left[ -1.2 \left( \frac{u'_e}{s_0^0} \right)^{-0.3} \right] \left( \frac{\Delta_e}{\delta_0^0} \right)^{2/3}
\]
\[
(4.11)
\]
Finally, the efficiency function, $E$, is defined as the ratio between the wrinkling factor, $\Xi$, of laminar flame ($\delta_L = \delta_L^0$) to thickened flame ($\delta_L = \delta_L^1$):

$$E = \frac{\Xi |_{\delta_L = \delta_L^0}}{\Xi |_{\delta_L = \delta_L^1}} \geq 1 \quad (4.12)$$

where the subgrid scale turbulent velocity is evaluated as $u'_{\Delta e} = 2\Delta_x^2 \left| \nabla^2 (\nabla \times \pi) \right|$, where $\Delta_x$ is the grid size. This formulation provides an estimate of the subgrid scale velocity which is unaffected by dilatation (Colin et al., 2000). The filter size $\Delta_e$ may differ from $\Delta_x$. It was prescribe by Colin (Colin et al., 2000) to choose $\Delta_e$ at least $10 \Delta_x$.

**4.2.2 Power-Law Flame Wrinkling Model**

This was proposed by Charlette et al. (2002). The main idea behind this analysis is to relate flame surface area (or reaction rate) to a cutoff length which limits wrinkling at the smallest length-scales of the flame. The cutoff scale is then related to the production of flame surface. The surface-producing flame stretch is then evaluated in terms of various parameters, and various important limiting behaviors. Based on the relevant asymptotic behavior, useful fits to the flame stretch and sub-grid flame velocity are proposed. Considering these hypothesis, the wrinkling function $E$ due to the flame wrinkling is given as:

$$E = \left(1 + \min \left[ \frac{\Delta_e}{\delta_L^0}, \Gamma \frac{u'_{\Delta e}}{s_L^0} \right] \right) \alpha \quad (4.13)$$

where the fits are defined as follows:

$$\Gamma \left( \frac{\Delta_e}{\delta_L^0}, \frac{u'_{\Delta e}}{s_L^0}, \text{Re}_{\Delta} \right) = \left[ \left( f_u^{-a} + f_{\Delta}^{-a} \right)^{-1/a} + f_{\text{Re}}^{-b} \right]^{-1/b} \quad (4.14)$$

$$f_u = 4 \left( \frac{27C_k}{110} \right)^{1/2} \left( \frac{18C_k}{55} \right) \left( \frac{u'_{\Delta e}}{s_L^0} \right)^2 \quad (4.15)$$

$$f_{\Delta} = \left[ \frac{27C_k \pi^{4/3}}{110} \times \left( \frac{\Delta_e}{\delta_L^0} \right)^{4/3} - 1 \right]^{1/2} \quad (4.16)$$

$$f_{\text{Re}} = \left[ \frac{9}{55} \exp \left( -\frac{3}{2} \frac{C_k \pi^{4/3} \text{Re}_{\Delta}^{-1}}{} \right) \right]^{1/2} \times \text{Re}_{\Delta}^{1/2} \quad (4.17)$$
where the constants $a$ and $b$ control the sharpness of the transitions between the asymptotic behaviors. The suggested values are

$$a = 0.60 + 0.20 \exp \left[ -0.1 \left( \frac{u'_{\Delta_e}}{s_L^0} \right) \right] - 0.20 \exp \left[ -0.01 \left( \frac{\Delta_e}{s_L^0} \right) \right], b = 1.4, \ C_k = 1.5,$$

$\Delta_e = F \delta_L^0$ and $Re_\Delta = \frac{4 \Delta_e u'_{\Delta_e}}{s_L^0}$. The exponent $\alpha$ determines the type of formulation. If $\alpha$ assumes to be constant value of 0.5 then it is regarded as 'non dynamic formulation', whereas if $\alpha$ is determined dynamically, then it is called as 'dynamic formulation' of power-law flame wrinkling model.

![Figure 4.1: Flame stretch for different length scale ratio. DNS results from Colin et al. (2000): cases An (o), Bn (□), Cn (◊). The Cn function [Eq. 4.32] (—), The modified Cn function [Eq. 4.33] (--)](image)

### 4.2.3 Dynamically Modified TF Model

The major issue with TF model is that it modifies the diffusion term (multiplying with a thickening factor $F$) throughout the whole computational domain, which may sometime lead to false prediction of species mass fraction in the regions where diffusion is relatively more important (like near wall). As a matter of fact, this effect may cause severe damage in case of inhomogeneous premixed or partially premixed combustion, especially in gas turbines where pure mixing (no chemical reaction), premixed and non-premixed zones may coexist, as the reciprocal
action of convection and diffusion in balance equation is being distorted.

To overcome this disadvantage, a dynamically thickened flame model has been initially developed at the CERFACS (Legier et al., 2000; Truffin et al., 2003). The sensor $\Omega$ detects the presence of the flame, and the thickening factor is modified in such a fashion that it becomes a local factor and acts only at the vicinity of the flame. It is expressed as:

$$\Omega = Y_F^T Y_O^{\text{loc}} \exp \left( -\Gamma \frac{T_a}{T} \right)$$  \hspace{1cm} (4.18)

where $\Gamma (<1)$ artificially decreases the activation temperature away from the flame front. Now the local thickening factor becomes

$$F_{\text{loc}} = 1 + (F - 1) \tanh \left( \beta \frac{\Omega}{\Omega_{\text{max}}} \right), \quad D_{i,\text{loc}} = D_i$$  \hspace{1cm} (4.19)

where $\Omega_{\text{max}}$ is the maximum of $\Omega$ (which can be evaluated analytically for a stoichiometric premixed flame) and $\beta$ controls the thickness of the transition layer between thickened and non-thickened regions. No specific values for the parameters ($\Gamma$ and $\beta$) have been prescribed and need to be tuned according to the physical problem.

Recently, Durand and Polifke (2007) came up with different expression for the sensor $\Omega$, based on the reaction progress variable ($c$). In this approach, $\Omega$ is defined as

$$F_{\text{loc}} = 1 + (F - 1) \Omega(c)$$  \hspace{1cm} (4.20)

$$\Omega(c) = 16 [c(1 - c)]^2$$  \hspace{1cm} (4.21)

$$c = 1 - \frac{Y_F}{Y_F^{\text{gen}}}$$  \hspace{1cm} (4.22)

Compared to equation 4.20, the equation 4.18 has smoother transition between the flame front and the zone close to it. The diffusion coefficient is finally modified according to the local thickening factor $F_{\text{loc}}$ as

$$D_{i,\text{loc}} = \frac{\mu}{S_c} EF_{\text{loc}} + (1 - F_{\text{loc}}) \frac{\mu_k}{S_{ct}}$$  \hspace{1cm} (4.23)
Hence, the transport equation 4.8 is modified according to these local functions as

\[
\frac{\partial \hat{Y}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \hat{p} \hat{u}_j \hat{Y}_i \right) = \frac{\partial}{\partial x_j} \left( \hat{p} \hat{E} \hat{F}_{loc} \frac{\partial \hat{Y}_i}{\partial x_j} \right) + \frac{\omega_i}{\hat{F}_{loc}} \tag{4.24}
\]

where the rest of the terms are evaluated according to standard TF model.

![Graph showing vortex efficiency functions](image)

Figure 4.2: Vortex efficiency functions: The function [Eq. 4.32] proposed by Colin et al. (2000) (—), The modified function [Eq. 4.33] (- - -).

### 4.2.4 Proposed Modified TF Model

This modified model is proposed by De and Acharya (2009). The efficiency function (E) in the modified TF model is proposed based on the direct numerical simulations (DNS) data set of flame-vortex interactions (Colin et al., 2000). The central ingredient of the TF model is the sub-grid scale wrinkling function $E$, which is defined by introducing a dimensionless flame surface wrinkling factor $\Xi$. The efficiency function (E) is defined by the ratio between the wrinkling factor, $\Xi$, of laminar flame ($\delta_L = \delta_L^0$) to thickened flame ($\delta_L = \delta_L^1$) as given in the equation 4.12. The factor $\Xi$ is the ratio of flame surface to its projection in the direction of propagation, and is defined as:

\[
\Xi \approx 1 + \beta \Delta_n |\langle \nabla \cdot n \rangle_s| \tag{4.25}
\]

where $\beta$ is a model constant, and $\langle \nabla \cdot n \rangle_s$ is the sub-grid scale surface curvature, which is
estimated from the balance equation of sub-grid scale flame surface density. Using the equilibrium assumption (Colin et al., 2000) of the sub-grid scale flame surface density (sub-grid flame stretch, \( \langle \kappa \rangle_s = 0 \)), which balances the production and destruction terms, the following relationship is obtained

\[
\langle \nabla \cdot u - nn : \nabla u \rangle_s \tilde{\Sigma} = -\langle w \nabla \cdot n \rangle_s \tilde{\Sigma}
\]  

(4.26)

where the destruction is approximated by assuming the flame front displacement speed to be equal to the unstrained laminar flame speed (\( s^0_L \)) as

\[-\langle w \nabla \cdot n \rangle_s \approx s^0_L \langle |\nabla \cdot n| \rangle_s \]  

(4.27)

The straining rate is approximated by the following expression

\[
\langle \nabla \cdot u - nn : \nabla u \rangle_s \approx \frac{u'_{\Delta e}}{\Delta e} \Gamma \left( \frac{\Delta e}{\delta^0_L}, \frac{u'_{\Delta e}}{s^0_L} \right)
\]  

(4.28)

where \( \Gamma \) is a fitting function that has to be defined. By combining Eqns. (4.25) - (4.28), the flame surface wrinkling factor, Eq. (4.25), can be written as

\[
\Xi = 1 + \beta \frac{u'_{\Delta e}}{s^0_L} \Gamma \left( \frac{\Delta e}{\delta^0_L}, \frac{u'_{\Delta e}}{s^0_L} \right)
\]  

(4.29)

- **Proposed Fitting Function** \( \Gamma \)

The fitting function, \( \Gamma \), can be expressed as a function of the global strain rate (\( \langle a_{\Gamma} \rangle_s \)), local filter size (\( \Delta_e \)), local sub-grid scale turbulent velocity (\( u'_{\Delta e} \)), and laminar flame speed (\( s^0_L \)), and is written as

\[
\Gamma = \frac{\langle a_{\Gamma} \rangle_s}{u'_{\Delta e}/\Delta e}
\]  

(4.30)

where the effective global strain rate is obtained by integrating the local strain rate over all the scales between the Kolmogorov scale and \( \Delta_e \). Hence, to model \( \Gamma \), the effective global strain rate needs to be estimated and is obtained by integrating the local strain rate induced due to a pair of vortices.

The strain rate \( S_r \) induced by a pair of vortices is expressed as

\[
S_r = C_n \left( \frac{r}{\delta^0_L}, \frac{u'}{\delta^0_L}, \frac{\langle u' \rangle}{r} \right)
\]  

(4.31)
To determine the effective strain rate $S_r$ induced by a pair of vortices of size $r$ and characteristics speed $v'$, the DNS data set (Colin et al., 2000) of classical flame-vortex interaction is used. The DNS data set includes the range $r/\delta_L^1 \in [1.2, 30]$ and $v_t/s^0_L \in [0.8, 8]$. The calculation of $S_r$ requires the function, $C_n$, needs to be defined and estimated as follows.

![Graph](image)

Figure 4.3: $\Gamma_n$ plotted for $l_t/\delta_L^1 = 100$. Solid lines (—) represent the results from the numerical integration of Eq. (4.37), Dashed lines (- - -) represent the proposed fit [Eq. 4.38].

The original $C_n$ function as proposed by Colin et al. (2000) is

$$C_n \left( \frac{r}{\delta_L^1}, \frac{v'}{s^0_L} \right) = \frac{1}{2} \left[ 1 + \text{erf} \left( 0.6 \ln \left( \frac{r}{\delta_L^1} \right) - \frac{0.6}{\sqrt{v'/s^0_L}} \right) \right]$$

(4.32)

A modified $C_n$ function with an additional correction term is invoked in the present work, as suggested by Charlette et al. (2002), and is based on a better parametric fit to the DNS data from Colin et al. (2000). This modified expression contains an additional term, Eq. (4.33), which ensures that the slow eddies (characteristic speeds less than $s^0_L/2$) do not stretch the flame. Hence, the fitting function, Eq.(4.30), which is a function of $s^0_L$, and derived from this modified expression, Eq.(4.33), also does not affect the flame front. Thus the flame surface wrinkling, Eq.(4.29), which inherently takes care of the interaction between the flame front and turbulence, is also not affected by the slow eddies. Therefore, in this modified TF model, the use of the
proposed fitting function, Eq. (4.33), has two consequences: (a) the eddies smaller than $F_0^{0.5}_{L}$ do not interact with the flame front, and (b) the eddies with characteristic speeds less than $s_{L}/2$ also do not stretch the flame front. These effects are parameterized in the sub-grid wrinkling factor, Eq. (4.29). The modified $C_n$ function is written as follows:

$$C_n \left( \frac{r}{\delta_L}, \frac{v'}{s_{L}} \right) = \frac{1}{2} \left[ 1 + \text{erf} \left( 0.75 \ln \left( \frac{r}{\delta_L} \right) - \frac{0.75}{v' / s_{L}} \right) \right] \times \frac{1}{2} \left[ 1 + \text{erf} \left( 3 \log \left( \frac{2v'}{s_{L}} \right) \right) \right]$$

(4.33)

The flame stretch, Eq. (4.31), and the expressions, Eqs. (4.32) and (4.33), for $C_n$ function are compared in Figs 4.1 & 4.2, respectively. The modified $C_n$ function shows better estimates of the flame stretch and to better fit the DNS results.

Charlette et al. (2002) used the similar expression for $C_n$ function, as given in Eq. (4.33), to model the sub-grid scale wrinkling factor and to come up with their proposed fitting function $\Gamma$. Their analysis was based on the relationship between strain rate and energy spectrum in homogeneous turbulence by making the association between length scale and wave number. In this work, we are following the previous work of Colin et al. (2000), where the effective global strain rate is obtained by integrating the effective strain rate due to a pair of vortices over all the length scales. However, we are using the modified $C_n$ function, Eq. (4.33), instead of Eq. (4.32) used in Colin et al. (2000). Considering the Kolmogorov cascade, the velocity $v'$ and length $r$ scales are related as

$$v' = \left( \frac{r}{l_t} \right)^{1/3} u' = \left( \frac{r}{\Delta_e} \right)^{1/3} u'_{\Delta_e}$$

(4.34)

where the velocity $u'$ corresponds to the turbulent integral length scale $l_t$. Hence, the corresponding strain rate becomes

$$\frac{v'}{r} = \left( \frac{l_t}{r} \right)^{2/3} \frac{u'}{l_t} = \left( \frac{\Delta_e}{r} \right)^{2/3} \frac{u'_{\Delta_e}}{\Delta_e}$$

(4.35)

The effective global strain rate integrated over all the scales between the Kolmogorov scale and
\( \Delta_e \) is given as

\[
\langle a_T \rangle_s = \frac{c_{ms}}{\ln 2} \int_{\text{scales}} \left( C_n \left( \frac{r}{\delta L}, \frac{v'}{s_L^0} \right) \left( \frac{v'}{r} \right) d \left[ \ln \left( \frac{l_t}{r} \right) \right] \right)
\]

(4.36)

where \( c_{ms} \) is considered as a model constant and the value is given as 0.28 by Yeung et al. (1990). Equation 4.36 is written as

\[
\langle a_T \rangle_s = \frac{c_{ms} u'_e \Delta_e}{\ln 2} \left( \frac{\Delta_e}{l_t} \right)^{2/3} \times \int_{\max[\ln(l_t/\Delta_e), 0]}^{(3/4) \ln(Re)} C_n \left( \frac{r}{\delta L} e^{-\left( \frac{l_t}{\Delta_e} \right)^{1/3} \frac{u'_e \Delta_e}{s_L^0} e^{-p/3}} \right) \times e^{(2/3)p} dp
\]

(4.37)

where \( \text{Re}_t = \frac{l_t u'}{\gamma} \approx 4(l_t/\delta_L^0)(u'/s_L^0) \) is turbulent Reynolds number. The integration is carried out for all the scales below \( \Delta_e \). The numerical integration is performed for the modified \( C_n \) function, Eq. (4.33), to calculate \( \Gamma \), Eq. (4.30), and compared with the fitting function \( \Gamma_n \), Eq. (4.38). Figure 4.3 shows that the \( \Gamma_n \) is in close agreement with the numerical integration of \( \Gamma \), Eq. (4.37). The fitting function \( \Gamma_n \) is given as

\[
\Gamma_n = \left[ -0.15 \exp \left( -0.15 \frac{\Delta_e}{\delta_L^1} \right) - 0.25 \exp \left( \frac{u'_e \Delta_e}{s_L^0} \right) + 0.85 \exp \left( -1.2 \left( \frac{u'_e \Delta_e}{s_L^0} \right)^{-0.3} \right) \right] \left( \frac{\Delta_e}{\delta_L^1} \right)^{2/3}
\]

(4.38)

Finally, the flame front wrinkling \( (s_T/s_L^0) \) is expressed as

\[
\Xi = \frac{s_T}{s_L^0} = 1 + \beta \frac{u'_e}{s_L^0} \Gamma_n
\]

(4.39)

where \( \text{Re}_t \) is the turbulent Reynolds number and the parameters are given in Eq. (??). For a given \( \text{Re}_t \) and the length scale ratio \( (\Delta_e/\delta_L^0) \), the velocity scale \( (u'_e/\delta_L) \) depends only on integral length scale ratio \( (l_t/\delta_L^0) \). It is observed that for a given \( \text{Re}_t \), \( s_T/s_L^0 \) decreases as the integral length scale increases and reaches to asymptotic values for higher length scale ratios. The function \( \Gamma \) represents the integration of the effective strain rate induced by all scales affected due to artificial thickening. The subgrid scale turbulent velocity is evaluated as \( u'_e = 2\Delta_x^3 (\nabla^2 (\nabla \times \pi)) \), where \( \Delta_x \) is the grid size. This formulation provides an estimate of the subgrid scale velocity which is unaffected by dilatation (Colin et al., 2000). The filter size \( \Delta_e \) may differ from \( \Delta_x \). It was prescribe by Colin (Colin et al., 2000) to choose \( \Delta_e \) at least 10 \( \Delta_x \).
The parameterization discussed above in both the original TF model (Colin et al., 2000) and the present modified TF model are derived based on the DNS data sets of 2D classical flame-vortex interaction results (Colin et al., 2000). Using a broader range of data sets that incorporate swirl, separation and other real effects for defining the TF model parameters would be appropriate, but such data sets that provide the needed turbulent-chemistry correlations are not available. However, other groups have used the original TF model to simulate large scale combustor problems with swirl and coaxial shear (Roux et al., 2005; Selle et al., 2004) and have achieved acceptably good results providing a basis of using the defined TF parameters for a broader class of problems.

In this work, the above mentioned models (TF model, Power-Law flame wrinkling model, dynamically modified model, Proposed modified TF model) have been implemented and tested.
Chapter 5 Flow Solver and Numerical Methods

A system of non-linear partial differential equations (PDE) are required to govern the flow field and others relevant models. For majority of practical applications, analytical solution of these non-linear partial differential are not possible. On the other hand, these PDE are numerically solved on a grid system by discretising into a system of algebraic equations. Due to large dimensionality and complexity, these algebraic system of equations are often solved iteratively. This chapter summarizes different aspects of flow solver and numerical methods used in this work, including general transport equations, averaged equations, discretization process, boundary conditions, solution methodologies and so on.

The most general form of transport equation is coordinate independent and expressed in vector notations (Jones, 2003). An arbitrary quantity \( \phi \) obeys a generalized conservation principle and has the form

\[
\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho u \phi) = \nabla \cdot (\Gamma \nabla \phi) + S
\]  

(5.1)

the terms on the l.h.s of the 5.1 are unsteady term, convective term, and on r.h.s are diffusion term, and general source term, respectively. The quantity \( \phi \) can be any number of quantities including mass fraction of chemical species, temperature, a velocity component, turbulent kinetic energy, turbulent dissipation rate. The exact form of source term \( S \), and the diffusion term \( \Gamma \), depends on the scalar quantity \( \phi \). The equation 5.1 can be expanded and then rearranged in a Cartesian coordinate system as

\[
\frac{\partial (\rho \phi)}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho w \phi - \Gamma \frac{\partial \phi}{\partial z} \right) = S
\]  

(5.2)

the equation 5.2 can be written in a compact form as

\[
\frac{\partial (\rho \phi)}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho u_i \phi - \Gamma \frac{\partial \phi}{\partial x_i} \right) = S
\]  

(5.3)

where the possible indices are number of spacial dimension in the flow. The three spacial
directions are \( x, y, z \) correspond to their respective velocity components \( u, v \) and \( w \). The equation 5.2 can also be written in terms of fluxes (described in details in the coming section) as

\[
\frac{\partial(Q)}{\partial t} + \frac{\partial}{\partial x} (E - E_v) + \frac{\partial}{\partial y} (F - F_v) + \frac{\partial}{\partial z} (G - G_v) = S \tag{5.4}
\]

where definitions of the conserved variable, \( Q \), and scalar fluxes, \( E, F \) and \( G \) (subscript \( v \) stands for viscous or diffusive parts) are understood from the comparison of equations 5.2 and 5.4. Similarly, the compact form (indicial notation) of equation 5.4 is

\[
\frac{\partial(Q)}{\partial t} + \frac{\partial}{\partial x_i} (E - E_v)_i = S \tag{5.5}
\]

the utility of transport equations are convenient when dealing with systems of transport equations.

In CFD calculations of turbulent reacting flows, a transport equation is required for each of the dependent variables \( \phi \) listed above, all of them are coupled with each other. When formulating sets of transport equations, it is often convenient to write dependent variables \( \phi_i \) as a vector of scalar dependent variable \( \Phi \). Here, the scalar quantity \( Q \) in equation 5.5 would become a vector of dependent variables, \( Q = [Y_i, u, v, w, T]^T \), where \( Y_i \) is the \( i \)th species mass fraction. Similarly, the convective and viscous flux quantities, \( E, E_v \), etc. and source term \( S \) would also become vector quantities.

### 5.1 Favre-averaged Governing Equations

The Favre-averaged N-S equations and turbulent mode equations are described in this section (Jones, 2003). A reduced notation introduced in the last section will be used here. For the time being, the conventional notation for partial derivatives will be more conveniently written using the shorthand notation \( \partial/\partial x \rightarrow \partial_z \). The \( i \)th species partial pressure, density, mass fraction, molecular weight and enthalpy is \( p_i, \rho_i, Y_i, W_i, h_i \) and the thermodynamic pressure, mixture density, velocity components and temperature are given by \( p, \rho, u, v, w \) and \( T \), respectively. Vector quantities are in bold type.

All species are assumed to obey an equation of state: \( p_i = \rho_iRT/W_i \). The equations are solved
simultaneously in a standard generalized coordinate systems with coordinate directions denoted by $\xi$, $\eta$ and $\zeta$. The appropriate vector quantities is of the form:

$$\partial_t \hat{Q} + \partial_\xi \left( \hat{E} - \hat{E}_v \right) + \partial_\eta \left( \hat{F} - \hat{F}_v \right) + \partial_\zeta \left( \hat{G} - \hat{G}_v \right) = \hat{H}$$  \hspace{1cm} (5.6)

The hats are used to represent the flux vectors, $\hat{E}$, $\hat{E}_v$, etc. in the generalized coordinate system and related to the flux vectors in the Cartesian $(x, y, z)$ frame:

\begin{align*}
\hat{Q} &= \frac{1}{J} Q \\
\hat{E} &= \frac{1}{J} (\xi_x E + \xi_y F + \xi_z G) \\
\hat{F} &= \frac{1}{J} (\eta_x E + \eta_y F + \eta_z G) \\
\hat{G} &= \frac{1}{J} (\zeta_x E + \zeta_y F + \zeta_z G)
\end{align*}

(5.7)

where $\xi, \eta$ and $\zeta$ are spacial coordinates in the generalized frame of reference.

5.1.1 Inviscid Fluxes

The conserved variable vector and inviscid fluxes in the Cartesian coordinate system are

\begin{align*}
Q &= [\rho Y_1, ..., \rho Y_N, \rho u, \rho v, \rho w, E_t]^T \\
E &= [\rho u Y_1, ..., \rho u Y_N, \rho u^2 + p, \rho uv, \rho uw, (E_t + p)u]^T \\
F &= [\rho v Y_1, ..., \rho v Y_N, \rho vw, \rho v^2 + p, \rho vw, (E_t + p)v]^T \\
G &= [\rho w Y_1, ..., \rho w Y_N, \rho w w, \rho w^2 + p, (E_t + p)w]^T
\end{align*}

(5.8)

The quantities $\rho, p, u, v, w$ and $Y_s$ denote density, pressure, Cartesian velocity components, and species mass fraction, respectively. The total energy is $E_t = \rho \left[ e + \frac{1}{2} (u^2 + v^2 + w^2) \right]$, where $e$ is specific internal energy.
5.1.2 Viscous Fluxes

The Cartesian viscous fluxes are written as

\[
E_v = [q_{x1}, \ldots, q_{xN}, \tau_{xx}, \tau_{xy}, \tau_{xz}, u\tau_{xx} + u\tau_{xy} + w\tau_{xz} + q_{xe}]^T \tag{5.9}
\]

\[
F_v = [q_{y1}, \ldots, q_{yN}, \tau_{yx}, \tau_{yy}, \tau_{yz}, u\tau_{yx} + v\tau_{yy} + w\tau_{yz} + q_{ye}]^T
\]

\[
G_v = [q_{z1}, \ldots, q_{zN}, \tau_{zx}, \tau_{zy}, \tau_{zz}, u\tau_{zx} + v\tau_{zy} + w\tau_{zz} + q_{ze}]^T
\]

with the stress components

\[
\tau_{xx} = 2\mu_e \partial_x u - \frac{2}{3} \mu_e (\partial_x u + \partial_y v + \partial_z w), \quad \tau_{xy} = \tau_{yx} = \mu_e (\partial_y u + \partial_z v) \tag{5.10}
\]

\[
\tau_{yy} = 2\mu_e \partial_y v - \frac{2}{3} \mu_e (\partial_x u + \partial_y v + \partial_z w), \quad \tau_{yz} = \tau_{zy} = \mu_e (\partial_y w + \partial_z v)
\]

\[
\tau_{zz} = 2\mu_e \partial_z w - \frac{2}{3} \mu_e (\partial_x u + \partial_y v + \partial_z w), \quad \tau_{zx} = \tau_{xz} = \mu_e (\partial_x u + \partial_y w)
\]

The mixture viscosity, \(\mu\), is obtained from the species component viscosities using Wilke’s mixing rule. The viscosity of each component in the gas mixture is computed using Chemkin (Kee, et al., 1995).

5.1.3 Energy Fluxes

The energy fluxes in the three coordinate directions are given by

\[
q_{xe} = k_e \partial_x T + \rho \sum_{s=1}^{N} h_s D_e \partial_x Y_s \tag{5.11}
\]

\[
q_{ye} = k_e \partial_y T + \rho \sum_{s=1}^{N} h_s D_e \partial_y Y_s
\]

\[
q_{ze} = k_e \partial_z T + \rho \sum_{s=1}^{N} h_s D_e \partial_z Y_s
\]

where \(T\) is temperature and \(k_e = k_t + C_{pm} \mu_t / Pr_t\), \(D_e = D_{sm} + \mu_t / Sc_t\) are effective thermal and molecular diffusivities, respectively. \(k_t, D_{sm}, \mu_t, Pr_t, Sc_t\) are molecular conductivity, molecular diffusivity of species \(s\), turbulent viscosity, turbulent Prandtl number and turbulent Schmidt number, respectively.
5.1.4 Mass Fluxes

The $s$th species mass diffusion fluxes are

$$q_{xs} = \rho \left( D_{sm} + \frac{\mu_t}{Sc_t} \right) \partial_x Y_s$$

(5.12)

$$q_{ys} = \rho \left( D_{sm} + \frac{\mu_t}{Sc_t} \right) \partial_y Y_s$$

$$q_{zs} = \rho \left( D_{sm} + \frac{\mu_t}{Sc_t} \right) \partial_z Y_s$$

The binary molecular diffusivity of species $s$ in the gas mixture is $D_{sm} = (1 - X_s) / \sum_{j \neq s}^N X_j / D_{sj}$.

The $s$th species molar fraction is $X_s$, $D_{sj}$ is the binary mass diffusivity between species $s$ and $j$, $Sc_t$ is turbulent Schmidt number.

5.1.5 Source Terms

Source terms arise from a number of physical processes. Some of the most common possibilities include source terms due to chemical reaction and gravitational of buoyancy effects.

The source term vector due to chemistry is $H_c = [S_1, ..., S_N, 0, 0, 0, 0]^T$, where the $s$th component of $H_c$ is the rate of change of the corresponding species due to reaction and is denoted by $S_s$. Each components, $S_s$ is the sum of all the reactions in a system containing $N_r$ chemical reactions.

$$S_s = W_s \sum_{r=1}^{N_r} \left[ \left( \gamma_{rs} - \gamma_{ss} \right) k_f \prod_{j=1}^N \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{s, j}} - k_b \prod_{j=1}^N \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{s, j}'} \right]$$

(5.13)

The individual species chemical source terms are discussed in one of the following sections.

Source term due to gravitational forces (buoyancy) are written as

$$H_b = [S_1, S_2, ..., S_N, \Delta \rho g_x, \Delta \rho g_y, \Delta \rho g_z, \Delta \rho (u g_x + v g_y + w g_z)]^T$$

while $g_{xi}$ is a body force components in the Cartesian frame of reference, and $\Delta \rho = \rho - \rho_r$, being $\rho_r$ as reference density.

The combined source vector due to the effects of all source terms is $H = H_c + H_b + H_{other}$.

5.1.6 Thermophysical Properties

The thermodynamic pressure is computed from Dalton’s law of partial pressures and the ideal
gas law:

\[ p = \sum_{s=1}^{N} p_s = \sum_{s=1}^{N} \frac{\rho_s}{W_s} RT \]  

(5.14)

The enthalpy of each species is computed as:

\[ h_s = h_{f_s}^0 + \int_{T_{ref}}^{T} C_{p_s} dT \]  

(5.15)

where \( R \) and \( T_{ref} \) are the universal gas constant and reference temperature for thermodynamics properties. \( W_s, C_{p_s}, h_s \) and \( h_{f_s}^0 \) are the molecular weight, specific heat, thermodynamic enthalpy and standard heat of formation of species \( s \), respectively. The species specific heats, \( C_{p_s} \), are evaluated using 4th order temperature polynomials and the specific heat of gas mixture is obtained by mass concentration weighting of each individual species. The enthalpy of the gas mixture is found similarly. As mentioned earlier, molecular viscosity, thermal conductivity and species diffusivities are computed using transport library of the Chemkin package (Kee et al., 1995). They can also be computed using the NASA thermodynamic curve fit format. (McBridge et al., 1993).

5.1.7 Chemistry and Kinetics Modeling

The chemical source elements, \( S_s \), of the chemical source term vector, \( H_c \), are handled as a set of \( N_R \) chemical reactions involving \( N \) chemical species in a standard Arrhenius fashion. The reaction equations are written in the general form

\[ \sum_{s=1}^{N} \gamma'_{rs} n_s \frac{k_{fr}}{k_{br}} \gamma''_{rs} n_s, \quad r = 1, 2, 3, ..., N_R \]  

(5.16)

where \( \gamma'_{rs} \) and \( \gamma''_{rs} \) are stoichiometric coefficients for the \( s \)th species appearing as a reactant in the \( r \)th forward and backward reactions, respectively, and \( n_s = \frac{\rho_s}{W_s} \), i the molar concentration of species \( s \). The rate of change of molar concentration of species \( s \) due to the \( r \)th elementary reaction step is

\[ (\partial_t n_s)_r = \left( \gamma''_{rs} - \gamma'_{rs} \right) \left( k_{fr} \prod_{j=1}^{N} (n_j)^{\gamma'_{rj}} - k_{br} \prod_{j=1}^{N} (n_j)^{\gamma''_{rj}} \right) \]  

(5.17)

where forward and backward reaction rate constants for the \( r \)th reaction step, \( k_{fr} \) and \( k_{br} \), are given
in terms of pressure-based equilibrium rate constants, \( k_{p_r} \), as

\[
k_{f_r} = k_{o_r}(T) \exp \left( \frac{-E_r}{RT} \right) \tag{5.18}
\]

\[
k_{b_r} = \frac{k_{f_r}}{k_{p_r}} (R_p T)^{\Delta n_r} \tag{5.19}
\]

where \( \Delta n_r = \sum_s (\gamma_{rs}^n - \gamma_{rs}^e) \) (s is summation over species), and the pressure-based gas constant, \( R_p = R/p_{atm} \), is defined as the universal gas constant divided by one atmospheric pressure.

In general, the reference reaction rate constant, \( k_{o_r}(T) \) for the \( r \)th reaction is a function of temperature and its value is determined from an empirical correlation as follows:

\[
k_{o_r}(T) = A_r T^{n_r} \tag{5.20}
\]

For gases in an equilibrium state, the partial pressure ratio of the species components is equal to the equilibrium constant, \( k_p \). At equilibrium, \( dG \mid_{p,T} = 0 \) and therefore only the Gibbs free energy of formation for each species is needed to determine the equilibrium constant. For a gas phase reaction of the form \( aA + bB \leftrightarrow cC + dD \), the equilibrium constant in terms of partial pressures (non-dimensionalized by atmospheric pressure) is defined as

\[
k_p = \left[ \frac{p_C}{p_A} \right]^c \left[ \frac{p_D}{p_B} \right]^d = \exp \left( -\frac{\Delta G^0}{RT} \right) \tag{5.21}
\]

where \( \Delta G^0 \) is defined as the standard free energy change. A relationship can extended to any general chemical reaction using the standard free energy change expressed in terms of molar Gibbs free energy (\( kcal/kg.kmol \)). The molar Gibbs free energy for the \( r \)th reaction is defined by the following expression

\[
\Delta G^0_r = \sum_{s=1}^{N} \gamma_{rs}^n \Delta g^0_{rs} - \sum_{s=1}^{N} \gamma_{rs}^e \Delta g^0_{rs} \tag{5.22}
\]

where the partial molar Gibbs free energy of the \( s \)th species in the \( r \)th reaction, \( \Delta g^0_{rs} \), consistent
with the polynomial fits for $C_p$ of MaBride et al. (1993) is:

$$
\Delta g^{0}_{rs} = \Delta h - T \Delta s
$$

$$
= C_{0_s} (1 - \ln T) T - C_{1_s} \frac{T^2}{2} - C_{2_s} \frac{T^3}{6} - C_{3_s} \frac{T^4}{12} - C_{4_s} \frac{T^5}{20} + C_{5_1_s} - C_{6_s} T
$$

where $C_{0_s}, C_{1_s}, C_{2_s}, C_{3_s}, C_{4_s}$ are identical to the constants in equation 5.15 and $C_{5_1_s}, C_{6_s}$ are 6th and 7th constants in the McBride database and represent the standard enthalpy, $h^{0}_{fr_s}$, and entropy $s^{0}_{fr_s}$ of formation, respectively.

The total Gibbs free energy exchange for the $r$th reaction is then computed as follows

$$
\Delta G^{0}_r(T) = \sum_{s=1}^{N} (\gamma''_{rs} - \gamma'_{rs}) \Delta g^{0}_{s}(T)
$$

The equilibrium reaction rate for the $r$th reaction is then computed as follows:

$$
k_{p_r} = \exp \left( \frac{\Delta G^{0}_r(T)}{RT} \right)
$$

The total rate change of mass concentration of species $s$ is obtained by summing up all the changes due to all $r$th reaction steps and multiplying by the molecular weight $w_s$ of species

$$
S_s = W_s \sum_{r=1}^{N_R} \left[ \left( \gamma''_{rs} - \gamma'_{rs} \right) \left( k_{f_r} \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma'_{rj}} - k_{b_r} \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma''_{rj}} \right) \right]
$$

5.2 LES Modeling

In this section, large eddy simulation (LES) modeling in curvilinear coordinates is described. In LES, the governing equations are spatially filtered with the filter width (proportional to grid size), to resolve the dynamics of the large scales, and the “universal” small scales are modeled. The dynamic modeling in curvilinear coordinate system is followed as given by Jordan (1999,2001, 2003 and 2003), Tafti (2005).

The turbulent eddy-viscosity is estimated as

$$
\nu_t = C \left( \frac{J}{3} \right)^{2/3} \left| \nabla \right|
$$

The filtered contravariant component of velocity is given as

$$
\mathbf{U}^j = k_x^i \mathbf{u} + k_y^j \mathbf{v} + k_z^j \mathbf{w}, \quad k = \xi, \eta, \zeta \quad \text{for } j = 1, 2, 3
$$
The filtered strain rate tensor is given as

$$\bar{S}_{ij} = \frac{1}{2} \left( (\bar{a}^k)_{j} \frac{\partial \bar{w}_i}{\partial \xi_k} + (\bar{a}^k)_{i} \frac{\partial \bar{w}_j}{\partial \xi_k} \right), \quad \text{where} \quad (\bar{a}^k)_{j} = J \frac{\partial \xi_k}{\partial x_j}$$  \hspace{1cm} (5.29)

where $J$ is the jacobian of transformation. The magnitude of the strain rate tensor is

$$|\bar{S}| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}.$$

### 5.2.1 Dynamic Procedure

The anisotropic subgrid ($-$) and subtest scale ($\hat{\cdot}$) stresses are formulated in terms Smagorinsky eddy viscosity model (Smagorinsky, 1963) as:

$$\hat{\tau}_{ij}^a = -2C(J)^{2/3}|\widehat{S}|\bar{S}_{ij}$$  \hspace{1cm} (5.30)

$$T_{ij}^a = -2C\alpha(J)^{2/3}\left|\widehat{S}\right|\widehat{S}_{ij}$$  \hspace{1cm} (5.31)

where $C$ is a model constant and assumed to be same in both subgrid and subtest level. $\alpha$ is square of the ratio of filter widths at subtest level to subgrid level. The Germano Identity (Germano et al., 1991) relates the SGS stresses at different filter levels in terms of the filtered fields as:

$$T_{i}^k = \hat{U}^k u_i - \hat{U}^k \hat{u}_i, \quad \tau_{i}^k = \hat{U}^k u_i - \hat{U}^k \hat{u}_i$$  \hspace{1cm} (5.32)

$$L_{i}^k = T_{i}^k - \tau_{i}^k = \hat{U}^k u_i - \hat{U}^k \hat{u}_i$$  \hspace{1cm} (5.33)

where $L_{i}^k$ is known as Leonard stress.

Therefore, using the Smagorinsky’s model for SGS terms, the Germano Identity becomes

$$L_{ij}^a = L_{ij} - \frac{1}{3} \delta_{ij} L_{kk} = -2C(J)^{2/3} \left( \alpha \left| \widehat{S}\right| \widehat{S}_{ij} - |\widehat{S}| \widehat{S}_{ij} \right)$$  \hspace{1cm} (5.34)

$$= -2C(J)^{2/3} M_{ij}$$

Using a least-squares approach by minimizing the error along the curvilinear lines, the constant $C$ is obtained as:

$$C = -\frac{1}{2} \frac{L_{ij}^a M_{ij}}{(J)^{2/3} M_{ij} M_{ij}}$$  \hspace{1cm} (5.35)
where the local value of $C$ is constrained to positive values.

5.3 Grid System

Finite volume formulation (FVM) in generalized coordinate system is used for the governing equations in this thesis work. The body-fitted multi-block structured grid is usually generated and used for simulations. The curvilinear grid is then transformed to a uniform, collocated grid in transformed reference frame, where finite difference method (FDM) approximations are used for the diffusion terms. In a collocated grid, the velocity components and scalars are defined at same location (i.e. cell center).

5.4 Discretization Methods

A second order low diffusion flux-splitting scheme (LDFSS) is used to discretized the convective terms in the momentum equation 5.6 (Edwards, 1997; Neaves et al., 2006; Mao et al., 2003). The terms $\hat{E}, \hat{F}, \hat{G}$ contain two parts: one is convective part and other one is pressure part. The LDFSS is applied to the cell interfaces in a FVM formulation. The inviscid flux being split into convective and pressure parts as the sum of left and right components and written as:

$$\Phi^k = \Phi^k_c + \Phi^k_p, \quad \Phi = \hat{E}, \hat{F}, \hat{G} \quad \text{for} \quad k = 1, 2, 3$$ (5.36)

where subscripts $c$ and $p$ stands for convective part and pressure part, respectively. At $i$th cell interface (i.e. $i + 1/2$ location) the splitted component is expressed as:

$$\Phi^k = (\Phi^k_c)_{i+1/2} + (\Phi^k_p)_{i+1/2}$$ (5.37)

$$(\Phi^k_c)_{i+1/2} = U^+ W_L + U^- W_R \quad \text{and} \quad (\Phi^k_p)_{i+1/2} = P_{i/2}$$ (5.38)

$$W_L = W_i + \frac{\Gamma_i \Psi_i}{2}, \quad W_R = W_{i+1} - \frac{\Gamma_{i+1} \Psi_{i+1}}{2}$$ (5.39)

with

$$\tilde{W} = [\tilde{u}, \tilde{v}, \tilde{w}, \tilde{T}, \tilde{p}]^T$$ (5.40)
\[
\Psi_i = \frac{(\Delta^2_+ + \epsilon^2) \Delta_- + (\Delta^2_- + \epsilon^2) \Delta_+}{\Delta^2_+ + \Delta^2_- + 2 \epsilon^2}
\] (5.41)

where \( \Delta_+ = \tilde{W}_{i+1} - \tilde{W}_i \) and \( \Delta_- = \tilde{W}_i - \tilde{W}_{i-1} \), \( \epsilon \) is a constant with small value.

\[
\Gamma_i = \kappa \left( 1.0 - \frac{|p_{i+1,j} - p_{i-1,j}|}{|p_{i+1,j} - p_{i-1,j}| + p_x} \right)
\] (5.42)

\[
\kappa = \begin{cases} 
0, & \text{1st order interpolation} \\
1, & \text{2nd order interpolation} 
\end{cases}
\]

To find \( U^+ \) and \( U^- \), the following calculations are done.

\[
U^+ = \tilde{a}_{1/2} \left[ M^+ - M_{1/2} \left( 1 - \frac{p_L - p_R}{2\rho_{r e f}} \right) \right]
\]

\[
U^+ = \tilde{a}_{1/2} \left[ M^- + M_{1/2} \left( 1 + \frac{p_L - p_R}{2\rho_{r e f}} \right) \right]
\] (5.43)

where \( \tilde{a}_{1/2} \) is the numerical speed of sound and \( M_{1/2} \) is the Mach number at the cell interface, and defines as following.

\[
M_{1/2} = \frac{1}{4} \beta_L \beta_R \left( \sqrt{\frac{1}{2} (M_L^2 + M_R^2) - 1.0} \right)^2
\] (5.44)

\[
\tilde{a}_{1/2} = \left[ \sqrt{(1 - M_{r e f}^2)u^2 + 4V_{r e f}^2} \right]_{1 + M_{r e f}^2}
\]

\[
M_{r e f}^2 = \frac{V_{r e f}^2}{a^2}
\]

\[
V_{r e f}^2 = \min \left( a^2, \max \left( \left| \vec{V} \right|^2, K \left| \vec{V}_\infty \right|^2 \right) \right)
\]

where \( V_{r e f} \) is reference velocity at cell interface, \( a \) is the effective speed of sound, \( \left| \vec{V} \right| \) is the local velocity magnitude, \( \left| \vec{V}_\infty \right| \) is the reference velocity and \( K \) is usually taken unity.

\[
M_{L,R} = \frac{u_{L,R}}{\tilde{a}_{1/2}} = \frac{1}{\tilde{a}_{1/2}} \frac{1}{\nabla \xi_i} \left( \xi_i u + \xi_i^j v + \xi_i^k w \right)
\] (5.46)

\[
\alpha_{L,R}^\pm = \frac{1}{2} \left[ 1.0 \pm sgn \left( M_{L,R} \right) \right], \quad \beta_{L,R} = - \max \left[ 0.0, 1.0 - int \left( \left| M_{L,R} \right| \right) \right]
\] (5.47)

\[
M_{(2)}^\pm = \pm \frac{1}{4} \left( M_{L,R} \pm 1 \right)^2, \quad M^\pm = \alpha_{L,R}^\pm \left( 1 + \beta_{L,R} \right) M_{L,R} - \beta_{L,R} M_{(2)}^\pm
\] (5.48)

The pressure splitting part is decomposed as:

\[
P_{1/2} = \frac{1}{2} \left[ p_L + p_R \right] + \frac{1}{2} \left( P^+ - P^- \right) \left( p_L - p_R \right) + \rho V_{r e f}^2 \left( P^+ + P^- - 1.0 \right)
\] (5.49)
\[ P^\pm = \alpha^\pm_{L,R} \left( 1 + \beta_{L,R} \right) - \frac{\beta_{L,R}}{2} \left[ 1.0 \pm M_{L,R} \right] \] (5.50)

All other spatial terms (i.e. diffusion terms) in the governing equations are discretized using second order central difference scheme. First order finite difference for the pseudo time derivative and second order finite difference for physical time derivatives are used, like

\[ \frac{\partial \phi}{\partial \tau} + \frac{\partial \phi}{\partial t} = \frac{\phi^{n+1} - \phi^n}{\Delta \tau} + \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} \] (5.51)

5.5 Boundary Conditions

The boundary conditions are used according to the physical problems. Several types of boundary conditions used in this thesis, few of them are briefly highlighted below.

5.5.1 Wall Boundary Condition

The solid may be solid or moving. In case of solid walls, no-slip boundary condition is used and wall is treated as an isothermal wall or adiabatic wall depending on the problem. Whereas, in case of moving wall, the moving wall boundary condition is used to specify the moving wall velocity.

5.5.2 Symmetric Boundary Condition

The symmetric boundary conditions are applied to solve 2D axis-symmetric problems, where the solutions variables are having same value on the both side of a surface.

5.5.3 Stress Free Boundary Condition

This boundary condition is usually used for the simulation of free shear layer flows.

5.5.4 Freestream Boundary Condition

This type of boundary condition is also used while doing some free shear layer flows with a huge computational domain, such as aerodynamic simulations.

5.5.5 Inlet Boundary Condition

There are different types of inlet conditions used in this code. One can use uniform inlet condition, one can use some inlet profile and so on.
5.5.6 **Turbulent Inlet Condition**

LES requires a time dependent turbulent inflow condition since the simulated turbulent flow is time dependent. Turbulent inflow condition is often generated in other numerical simulations or presumed following certain but limited measurement data. Several boundary conditions have been proposed so far by different researcher (Spalart, 1988; Lund et al., 1998; Klein et al., 2003). However, the most sample way to use some laminar profile (without any turbulent fluctuations) and allow the flow to develop, which requires a larger upstream passage from the region of interest. An alternative way is to add some kind of fluctuations to the laminar profile, like white noise with certain scaling. Accurate turbulent inflow conditions can be obtained from an auxiliary simulation (Akselvoll & Moin, 1996) or by using some periodic boundary conditions (Spalart, 1988). There are several alternative approaches available, however, none of them are exact though.

Two types of inlet conditions are used in this work. One way, it is interpolated from measured data & used with the inlet profile. Alternatively, a random flow generating technique (Smirnov et al., 2001) is used, for which the auxiliary data set is generated through another numerical simulation.

- **Random Inflow Generation Technique**

This method is a modified version of Kraichman’s technique. This method has the following steps:

1. Given an anisotropic velocity correlation tensor, \( r_{ij} \equiv \overline{u_i u_j} \) (generated from another simulation or taken from measured data) of a turbulent flow field \( \{ \overline{u_i(x, t)} \}_{i,j=1..3} \), an orthogonal transformation tensor \( a_{ij} \) is found that would diagonalize the \( r_{ij} \), such as

\[
a_{mi} a_{nj} r_{ij} = \delta_{mn} c_{(n)}^2, \quad a_{ik} a_{kj} = \delta_{ij}
\]

(5.52)

Due to this operation, \( a_{ij} \) and \( c_n \) become a known functions of space. Coefficients \( c_n = \{ c_1, c_2, c_3 \} \) play the role of turbulent fluctuation components \( (u', v', w') \) in the new
transformed coordinate systems.

(2) Generating the transient flow filed \( \{v_i(x_j, t)\}_{i,j=1,3} \) using the following operations:

\[
v_i(\vec{x}, t) = \sqrt{\frac{2}{N}} \sum_{n=1}^{N} \left[ p_i^n \cos \left( k_j x_j + \omega_n t \right) + q_i^n \sin \left( k_j x_j + \omega_n t \right) \right]
\]  

(5.53)

where \( x_j = \frac{x_j}{l}, \tau = \frac{\tau}{\tau}, k_j^n = k_j^n \frac{c}{v_{(j)}}, \) and \( p_i^n = \varepsilon_{ijm} \xi_{jn} \xi_{jm}, q_i^n = \varepsilon_{ijm} \xi_{jn} \xi_{jm}, \) \( \xi_{jn}, \xi_{jm}, \omega_n \in N(0, 1), \) \( k_j^n \in N(0, 1/2), \) with \( l, \tau \) as turbulent length and time scales, \( \varepsilon_{ijk} \) as permutation tensor and \( N(M, \sigma) \) as normal distribution with mean \( M \) and standard deviation \( \sigma \).

(3) Finally, applying the scaling and orthogonal transformations to the flow field generated through previous step, a new transient flow field is generated

\[
w_i = c_{(i)} v_{(i)}, \quad u_i = a_{ik} w_k
\]  

(5.54)

This procedure needs an input correlation tensor of the original flow field and turbulent length & time scales, which can easily obtained from steady-state RANS calculation or experimental data.

### 5.5.7 Outflow Condition

A convective outflow condition is used in this work. The same condition was used in previous LES of a confined co-annular jet flow (Akselvoll & Moin, 1996), diffusion flames (Pitsch & Steiner, 2000), and premixed flames (Pitsch & Duchamp, 2002). The expression for the convective outflow is given as:

\[
\frac{\partial \tilde{\phi}}{\partial t} + U_{con} \frac{\partial \tilde{\phi}}{\partial n} = 0
\]  

(5.55)

where \( U_{con} \) is the mean outflow velocity integrated across the outlet plane, \( n \) is the normal to outflow surface.

### 5.6 Solution Methodologies

#### 5.6.1 Preconditioning

Low Mach number preconditioning is done to effectively rescale the acoustics scale to match that of convective scales (Weiss & Smith, 1994). A pseudo time derivative of the dependent
variable vector is added to the transport equation 5.6 as follows

\[ \Gamma \frac{\partial \hat{U}}{\partial t} + \frac{\partial \hat{Q} + \partial \hat{E}}{\partial t} + \partial \hat{v} \left( \hat{\mathcal{E}} - \hat{\mathcal{E}_v} \right) + \partial \hat{v} \left( \hat{\mathcal{F}} - \hat{\mathcal{F}_v} \right) + \partial \hat{v} \left( \hat{\mathcal{G}} - \hat{\mathcal{G}_v} \right) = \hat{H} \]  

(5.56)

The dependent variables and preconditioning matrix are defined by

\[ \hat{U} = \frac{1}{J} \left[ p_1, p_2, \ldots, p_N, u, v, w, T \right]^T \]  

(5.57)

\[ \Gamma = \begin{bmatrix}
\frac{W_1}{RT} + \Theta Y_1 & \Theta Y_1 & \ldots & \Theta Y_1 & 0 & 0 & 0 & -\frac{\rho_1}{T} \\
\Theta Y_2 & \frac{W_2}{RT} + \Theta Y_2 & \ldots & \Theta Y_2 & 0 & 0 & 0 & -\frac{\rho_2}{T} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
\Theta Y_N & \Theta Y_N & \ldots & \frac{W_N}{RT} + \Theta Y_N & 0 & 0 & 0 & -\frac{\rho_N}{T} \\
u \left( \frac{W_1}{RT} + \Theta \right) & u \left( \frac{W_2}{RT} + \Theta \right) & \ldots & u \left( \frac{W_N}{RT} + \Theta \right) & \rho & 0 & 0 & -\frac{\upsilon_\rho}{T} \\
v \left( \frac{W_1}{RT} + \Theta \right) & v \left( \frac{W_2}{RT} + \Theta \right) & \ldots & v \left( \frac{W_N}{RT} + \Theta \right) & 0 & \rho & 0 & -\frac{\upsilon_\rho}{T} \\
w \left( \frac{W_1}{RT} + \Theta \right) & w \left( \frac{W_2}{RT} + \Theta \right) & \ldots & w \left( \frac{W_N}{RT} + \Theta \right) & 0 & 0 & \rho & -\frac{\upsilon_\rho}{T} \\
\alpha_1 & \alpha_2 & \ldots & \alpha_N & \rho u & \rho v & \rho w & \rho \left( C_{pm} - \frac{H}{T} \right)
\end{bmatrix} \]  

(5.58)

with

\[ V_{ref}^2 = \min \left[ a^2, \max \left( \frac{|\vec{V}|}{K}, \frac{|\vec{V}_\infty|}{\left| \frac{\vec{V}}{\sqrt{a^2}} \right|} \right) \right] \]  

(5.59)

\[ \Theta = \frac{1}{V_{ref}} - \frac{1}{\alpha^2} \]

\[ \alpha_s = H \left( \Theta + \frac{W}{RT} \right) - 1 \]

where \( H \) is the enthalpy per unit mass, \( a \) is the effective speed of sound, \( |\vec{V}| \) is the local velocity magnitude, \( |\vec{V}_\infty| \) is the reference velocity and \( K \) is usually taken unity.

Equation 5.56 represents \( N + 4 \) transport equation for a chemically reacting mixture of \( N \) species gases, in addition to three momentum and one energy equation, in a generalized curvilinear coordinate system. The equations are coupled and the resulting set is closed using an appropriate equation of state.

For incompressible flow, the characteristic velocity, \( V \) of the flow becomes small compared to the sound speed \( a \) (i.e. for low Mach numbers, \( M = V/a \)), hence, the compressible Navier-Stokes equation set becomes stiff due to large variations in system eigenvalues. In addition to that, the pressure term in the momentum equations becomes singular in the incompressible (zero Mach number) limit, resulting in solution inaccuracies due to excessively large round-off errors.
Theoretically, these problems can be circumvented by using a large CFL number and implicit solution schemes. However, in reality, numerical discretization errors necessitate CFL numbers which result in intolerable rates of convergence. At low Mach numbers, there are large disparities among CFL numbers based on each eigenvalue. The pseudo-time derivative term containing the preconditioning matrix in equation 5.56 has the effect of scaling the eigenvalues such that each equation is properly conditioned. The pseudo-time term also provides a coupling between the pressure and velocity fields, since the pressure does not appear in the species continuity equations.

The iterative solution procedure involves driving the pseudo-time derivatives of pressure in the continuity equations to zero yielding the steady-state solution for steady calculations or the solution at the current physical time in transient calculations.

5.6.2 Algorithm

The $\xi$, $\eta$ and $\zeta$ directions are discretized using $j$, $k$ and $l$, respectively. Using $p$ as a pseudo time index and $n$ as physical time index ($\pm$ implies $p + 1$), the discretized form of equation 5.56 becomes

\[
\frac{1}{\Delta x} \left( \frac{\tilde{U}^p_{i+} - \tilde{U}^n_{i+}}{\frac{\Delta t}{\Delta x}} \right) + \frac{1}{\Delta t \Delta x} \frac{3}{3} \left( \tilde{Q}^p_{i+} - 4\tilde{Q}^n_{i+} + \tilde{Q}^{-n}_{i+} \right) + \left[ \tilde{E} - \tilde{E}_{v}\right]_{j+} - \left[ \tilde{E} - \tilde{E}_{v}\right]_{j-} + \left[ \tilde{F} - \tilde{F}_{v}\right]_{k+} - \left[ \tilde{F} - \tilde{F}_{v}\right]_{k-} + \left[ \tilde{G} - \tilde{G}_{v}\right]_{l+} - \left[ \tilde{G} - \tilde{G}_{v}\right]_{l-} = \tilde{H}^{p+n+}_{i+} \tag{5.60}
\]

The solution vector is the change in the dependent variable vector and is defined as:

\[\delta \tilde{U}^p_{i+} = \tilde{U}^p_{i+} - \tilde{U}^n_{i+}.\]

Denoting $\tilde{P}_{i\pm}$ as a generic numerical approximation to the fluxes $\tilde{E}, \tilde{F}, \tilde{G}$ for $i = j, k, l$ respectively. The linearizations for the inviscid flux, viscous flux, conserved variable and source term vectors, respectively are:

\[
\begin{align*}
\tilde{P}_{i\pm}^{p+n+} &= \tilde{P}_{i\pm}^{p+n+} + \partial_{\tilde{U}} \tilde{P}_{i\pm} \delta \tilde{U}_{i\pm}^{p+n+} \\
\tilde{Q}_{i\pm}^{p+n+} &= \tilde{Q}_{i\pm}^{p+n+} + \partial_{\tilde{U}} \tilde{Q}_{i\pm} \delta \tilde{U}_{i\pm}^{p+n+} \\
\tilde{H}_{i\pm}^{p+n+} &= \tilde{H}_{i\pm}^{p+n+} + \partial_{\tilde{U}} \tilde{H}_{i\pm} \delta \tilde{U}_{i\pm}^{p+n+}
\end{align*}
\tag{5.61}
\]

The Jacobian matrices $\partial_{\tilde{U}} \tilde{P}, \partial_{\tilde{U}} \left( \tilde{P}_{i\pm} \right), \partial_{\tilde{U}} \tilde{Q}_{i\pm}$, and $\partial_{\tilde{U}} \tilde{H}_{i\pm}$ are given in Appendix A. Using the linearization of equation 5.61, the matrix equation for $\delta \tilde{U}$ at the $p_+$ pseudotime iteration of the $n_+$

93
physical time level is given as:

\[
\left( \frac{1}{\Delta x} + \partial_{U} \tilde{H}_{i} + \frac{1.5}{\Delta t} \partial_{U} \tilde{Q}_{i} \right) \delta \tilde{U}_{i}^{p,n+} \\
+ \left[ \partial_{U} \tilde{E} - \partial_{U} \tilde{E}_{v} \right]_{j} \delta \tilde{U}_{j}^{p,n+} - \left[ \partial_{U} \tilde{E} - \partial_{U} \tilde{E}_{v} \right]_{j} \delta \tilde{U}_{j}^{p,n+} \\
+ \left[ \partial_{U} \tilde{F} - \partial_{U} \tilde{F}_{v} \right]_{k} \delta \tilde{U}_{k}^{p,n+} - \left[ \partial_{U} \tilde{F} - \partial_{U} \tilde{F}_{v} \right]_{k} \delta \tilde{U}_{k}^{p,n+} \\
+ \left[ \partial_{U} \tilde{G} - \partial_{U} \tilde{G}_{v} \right]_{l} \delta \tilde{U}_{l}^{p,n+} - \left[ \partial_{U} \tilde{G} - \partial_{U} \tilde{G}_{v} \right]_{l} \delta \tilde{U}_{l}^{p,n+} = RHS^{p,n+}
\]

(5.62)

where

\[
RHS^{p,n+} = - \left\{ \left[ 1.5 \tilde{Q}_{i}^{p,n+} - 2 \tilde{Q}_{i}^{n+} + 0.5 \tilde{Q}_{i}^{n} \right] / \Delta t \\
+ \left[ \tilde{E} - \tilde{E}_{v} \right]^{p,n+} - \left[ \tilde{E} - \tilde{E}_{v} \right]^{p,n+} \\
+ \left[ \tilde{F} - \tilde{F}_{v} \right]^{p,n+} - \left[ \tilde{F} - \tilde{F}_{v} \right]^{p,n+} \\
+ \left[ \tilde{G} - \tilde{G}_{v} \right]^{p,n+} - \left[ \tilde{G} - \tilde{G}_{v} \right]^{p,n+} + \tilde{H}_{i}^{p,n+} \right\}
\]

(5.63)

Equation 5.63 is solved using ILU scheme.

5.7 Parallel Communication

The system of equations are solved in a zonal manner. Usually, the solution domain is divided into an arbitrary number of grid zones, Z, and the partitioning of these domains among an arbitrary number of processes, P, with the requirement that P ≤ Z, is done through parallel solution strategy. Each process solves its pre-assigned portion of the domain, subject to the boundary conditions for that part of the domain. Domain boundaries which are not physical boundaries share their data with the neighboring domains, either by in-memory data transfer when the domains reside on the same process or through inter-process data transfers when they reside on different processes. The inter-process communication is accomplished via MPI protocol (Gropp et al., 1999).

Parallel efficiency is highly dependent on the physical problem and can be controlled by the user during the grid generation step. It is expected that applications using zones of approximately the same size will exhibit a higher level of parallel efficiency due to uniform communication and computation load. Data communication on adjacent block boundaries is taken place during every solution iteration. The amount of information needed to update these inter-block values is kept to
a minimum. The parallel setup routines precompute the memory addresses of both the sources
and destinations of all data transfer events, whether in-memory or inter-process. Using these
precomputed addresses, only the data values must be exchanged during each iteration, minimizing
the communications overhead.

The computational effort is usually divided among each process in such a way that each
process completes its work in about the same length of time. An efficient parallel computation
can be achieved through proper load balancing, which can be ensured by keeping the size of
solution zones fairly uniform and the number of solution zones significantly larger than the
number of processes. However, parallel performance is not solely dependent on computational
load balancing. It also depends on the inter-processor communications, which increase with the
number of processes assigned to the problem. Moreover, if the sizes of the zones are made too
small, the amount of data transferred, relative to the amount of CPU work required, will also
increase. Assignment of grid zones to a user-defined number of processes is automatic and is
accomplished using METIS (Karypis and Kumar. 1998). More detailed information is available
in the literature by Harvey et al. (2003).
Chapter 6 LES of Turbulent Flows: Validation Studies

In order to validate the Large Eddy Simulation (LES) code, a number of validation benchmarks are undertaken for general configurations relevant to the geometry of interest.

6.1 Flows Over Backward Facing Step

Many engineering applications, such as flow in diffusers, combustors, channels with sudden expansion, flow over airfoils, are turbulent in nature and encounter separation and reattachment of such flows. Due to wide applicability, this kind of flows have received much attention over the past few decades and numerous experimental (Kuehn, 1980; Durst & Tropea, 1981; Ötügen, 1991, Driver & Seeegmiller, 1985) and theoretical (Armaly et al., 1983, Durst & Pereira, 1988; Steffen, 1993; Le et al., 1997) studies have been carried out and reported.

6.1.1 Flow Configuration

To validate the numerical methods, the flows over backward facing step have been simulated and compared with the experiments for different Reynolds numbers. Figure 6.1 shows the schematic of such flow

![Figure 6.1: A schematic of backward-facing step (BFS) flow configuration](image-url)
configuration in 3D simulations. At the inlet logarithmic velocity profile is used, whereas convective boundary condition is used at the exit boundary. No slip boundary conditions are used at the walls and in the spanwise direction, symmetric boundary condition is used.

6.1.2 \( \text{Re}_h \approx 5000 \)

The experimental study was carried out by Jovic & Driver (1994). The Reynolds number is calculated based on free stream velocity and step height. The computational details are given in the Table 6.1. The physical time step is taken 0.025 & 0.015 seconds for coarse and fine mesh respectively. The averaging of the turbulent flow field is performed over 50 flow-through times in the computational domain. The reattachment length is found reasonable compared to experimental value of \( X_r/h=6.0 \).

Table 6.1: Computational parameters for BFS at low Reynolds number

<table>
<thead>
<tr>
<th>Cases</th>
<th>( L_x )</th>
<th>( L_y )</th>
<th>( L_z )</th>
<th>Gid points</th>
<th>( X_r/h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>30h</td>
<td>10h</td>
<td>6h</td>
<td>4h</td>
<td>0.22M</td>
</tr>
<tr>
<td>Fine</td>
<td>30h</td>
<td>10h</td>
<td>6h</td>
<td>4h</td>
<td>1.38M</td>
</tr>
</tbody>
</table>

6.1.2.1 Results

Computed results are plotted against experimental data at different axial locations. Figures 6.2–6.6 show the mean axial velocity, latitudinal velocity and Reynolds stress profiles at different axial locations including the recirculation, reattachment and recovery regions. Mean velocity profiles are in good agreement with the experiments in recirculation and recovery regions as well. However, Reynolds stress predictions exhibit some discrepancies in both the regions. Essentially, the turbulent activities are dominant in the recirculation regions and decay gradually in the downstream locations, where the inner layer Reynolds stresses behave exactly like an ordinary turbulent boundary layer, whereas in the outer layer it decays slowly due to the presence of large eddies which are generated in the upstream shear layer. The coarse mesh shows better agreement in recirculation region, where the fine mesh slightly overpredicts the stresses. However, fine mesh shows better agreement in recovery region, where coarse mesh underpredicts. These discrepancies
may be partly due to numerical dissipation. The overall data predictions are in good agreement with the experiments.

Figure 6.2: Mean axial velocity profiles(BFS, $Re_h \approx 5000$): symbols (○) are experimental data, solid lines (—) are coarse mesh data, dashed lines (– –) are fine mesh data

6.1.3 $Re_h \approx 37420$

The experimental study was carried out by Driver& Seegmiller (1985). The Reynolds number is calculated based on free stream velocity and step height. The computational details are given in the Table 6.2. The physical time step is taken 0.01& 0.005 seconds for coarse & fine mesh respectively. The averaging of the turbulent flow field is performed over 40 flow-through times in the computational domain. The reattachment length is found reasonable compared to experimental value of $X_r/h=6.26$. 
Table 6.2: Computational parameters for BFS at high Reynolds number

<table>
<thead>
<tr>
<th>Cases</th>
<th>$L_x$</th>
<th>$L_y$</th>
<th>$L_z$</th>
<th>Gid points</th>
<th>$X_r/h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>75h</td>
<td>15h</td>
<td>9h</td>
<td>4h</td>
<td>0.59M</td>
</tr>
<tr>
<td>Fine</td>
<td>75h</td>
<td>15h</td>
<td>9h</td>
<td>4h</td>
<td>2.21M</td>
</tr>
</tbody>
</table>

Figure 6.3: Mean vertical velocity profiles (BFS, $Re_h \approx 5000$): Legend-See Fig. 6.2
Figure 6.4: Reynolds stress ($u'v'$) profiles (BFS, $Re_h \approx 5000$): Legend-See Fig. 6.2
Figure 6.5: Reynolds stress ($v'^2$) profiles (BFS, $Re_h \approx 5000)$: Legend-See Fig. 6.2
Figure 6.6: Reynolds stress (-u’v’) profiles (BFS, Re_h ≈ 5000): Legend-See Fig. 6.2
Figure 6.7: Mean axial velocity profiles (BFS, $Re_h \approx 37420$): Legend-See Fig. 6.2
Figure 6.8: Turbulent kinetic energy profiles (Re_h ≈ 37420): Legend—See Fig. 6.2
Figure 6.9: Turbulent shear stress profiles ($Re_h \approx 37420$): Legend—See Fig. 6.2
6.1.3.1 Results

Computed results are plotted against experimental data at different axial locations. Figures 6.7-6.9 show the mean axial velocity, turbulent kinetic energy, and turbulent shear stress profiles at different axial locations including the recirculation, reattachment and recovery regions. The overall mean axial velocity predictions are in good agreement with the experiments. However, some discrepancies have been observed in turbulent kinetic energy predictions, especially in the neighborhood of the reattachment regions. The peak value of the turbulent kinetic energy, in the recirculation region, is consistently predicted far away from the wall. The data at the location X/H=2.5 is found to be the most irregular. The remaining kinetic energy profiles, in recovery regions, are in reasonably good agreement with the experiments. Similar trends have been observed in the prediction of turbulent shear stress profiles. In the recirculation regions, the peak values are always overpredicted and located far away from the wall. However, in the downstream locations (recovery regions) the predictions are in good agreement. As the grid resolution is increased, no substantial differences have been observed in data predictions, that confirms the correct implementation of LES modeling part.

6.2 Isothermal Swirling Flow in a Confined Geometry

Confined swirling flows are of great interest due its widely used practical applications, especially in combustion chambers where the flame-turbulence interaction becomes significant in the presence of flow instabilities. These instabilities are often associated with the vortex breakdown phenomenon, which is caused due to existence of the inlet swirl in the system, makes the problem more complicated. The swirling motion at the inlet is usually generated using some guide vanes, inlet tangential flow injections, or by other means. The swirling flows are not only a time dependent phenomena but also three dimensional in nature. Hence, that necessiates the comprehensive computations of such flows for better understanding of the flow physics. Although an extensive research efforts, such as theoretical (Wang et al., 1996; Fernadez-Feria et al., 1996),
experimental (Billant et al., 1998; Panda et al., 1994), numerical (Kubo et al., 1975; Nejad et al., 1989; Weber et al., 1990) have been made so far, still remain a challenging problem to the research community.

6.2.1 Flow Configuration

The LES simulations have been performed to validate the confined swirling flows for the experimental configuration of Dellenback et al. (1986, 1988) at Reynolds number Re=30000. Figure 6.10 shows the schematic of the flow configuration in 3D simulations. At the inlet swirling inlet condition for velocity is used, whereas convective boundary condition is used at the exit boundary. The walls are treated as no slip boundary. The swirl number (S) for the present configuration is 0.6, and S is defined as

$$S = \frac{1}{R} \frac{\int_0^R r^2U_xW \, dr}{\int_0^R rU_x^2 \, dr}$$  \hspace{1cm} (6.1)$$

where $U_x$ is the axial velocity component and $W$ is the azimuthal velocity component, and $R$ is the radius of the nozzle.
Figure 6.11: Mean axial velocity profiles for confined swirling flow (S=0.6): symbols (Δ) are experimental data, solid lines (—) are coarse mesh data, dashed lines (---) are fine mesh data
Figure 6.12: Mean azimuthal velocity profiles for confined swirling flow (S=0.6): Legend-See Fig. 6.11
Figure 6.13: Axial components of Reynolds stresses for confined swirling flow (S=0.6): Legend—See Fig. 6.11
Figure 6.14: Azimuthal components of Reynolds stresses for confined swirling flow (S=0.6): Legend—See Fig. 6.11
6.2.2 Results

The Reynolds number (Re) for the test case is 30000 and swirl number (S) is 0.6. Two different grids are used for computations: one is coarse mesh with 0.31M grid points and other one is fine mesh with 2.29M grid points. The physical time step is taken 0.10 and 0.005 seconds for coarse and fine mesh respectively.

Figures 6.11-6.14 show the time averaged mean axial velocity, azimuthal velocity as well as Reynolds stresses profiles at different axial locations. Due to swirling motion, the center fluid is moved outward and resulting the decrease of the axial velocity in the inner part near the axis and increase in the outer part. Moreover, the sudden expansion at the backward-facing step wall introduces another deceleration to the existing low speed axial velocity at the axis. These two effects combinedly form an ’internal recirculation zone (IRZ)’ as shown in Figure6.11. At the downstream locations the axial and azimuthal velocity profiles become smoother. At X/D > 3.0, both the axial and azimuthal velocity components are significantly lower than the peak values at the upstream (Fig 6.11-6.12), and this is caused due to the inherent property of swirling flow (high spreading rate of momentum). In fact, this property is often used in the combustion system to enhance the mixing.

Figure 6.13 shows the axial components of the Reynolds stress profile. At X/D =0.25, two peaks are observed, and these two peaks are formed due to interaction of two strong shear layers: one is near the bakward-facing step walls, and the other is due to IRZ. The IRZ shear layer is observed at the boundary of the IRZ, where most of the kinetic energy is produced. In the first few locations, the axial and azimuthal components of the Reynolds stresses differ significantly, that implies that the turbulence in backward-facing step region is highly anisotropic. After the recirculation zone (X/D=2.0-3.0), the turbulence becomes isotropic. It is evident from the Figures 6.13-6.14 that the decay rate of turbulent fluctuation in swirling flows is higher than that of
nonswirling flows. Apart from the small discrepancies found in predicting the peak values of the Reynolds stresses, the overall agreement for both the coarse and fine mesh results is good.
Chapter 7 LES of Turbulent Premixed Combustion in a Bunsen Burner *

To assess the performance of Thickened flame approach, simulations of premixed flame are compared with the piloted premixed stoichiometric methane-air flame data (Chen et al., 1996) for Reynolds numbers Re = 24,000 (flame F3) and Re=52000 (flame F1). In the Thickened Flame model, the flame front is artificially thickened to resolve it on the computational LES grid. Since the flame front is resolved, the combustion chemistry can be incorporated directly without closure approximations for the reaction rate. The response of the thickened flame to turbulence is taken care of by incorporating an efficiency function in the governing equations. The efficiency function, which is also known as a sub-grid flame wrinkling parameter, is a function of local turbulence and of the premixed flame characteristics, such as laminar flame speed and thickness. Two variants of the thickened flame model, the power-law wrinkling model and the dynamic thickened flame model, have also been considered. Reasonable agreement is found when comparing predictions with the experimental data and with computations reported using a probability distribution function (PDF) modeling approach (Lindstedt et al., 2005) and G-equation approach (Duchamp et al., 2000, 2001, 2002).

In an earlier LES study, an alternative approach using a level-set flamelet model is presented by Duchamp et al. (2000), where they applied the methodology to examine the Bunsen flame at a Reynolds number Re=24000 (flame F3). The reported results show reasonably good agreement for the flow field and turbulent kinetic energy. However, the jet spreading rate and the turbulent kinetic energy in the shear layer are always over-predicted while the mean temperature profiles are shifted radially towards the centerline. No species concentration data are presented.

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In the context of RANS based simulations, Prasad and Gore (1999) reported a comparative study of different flame surface density models for Re=24000 (flame F3). They presented the mean flow and temperature profiles, but no species mass fraction and turbulent kinetic energy data were reported. In later studies, Lindstedt and Vaos (2006) reported the use of a PDF transport approach at Re=24,000 and 52,000, and showed good agreement with data, while Hermann (2006) used a level set flamelet model with different turbulence levels. Their studies show overall good agreement with the measured data except for discrepancies in the turbulent kinetic energy predictions as well as CO predictions.

7.1 Flow Configuration and Computational Details

The configuration of interest in the present work is the Bunsen burner geometry investigated by Chen et al. (1996), is shown in Figure 7.1. The flame is a stoichiometric premixed methane-air flame, stabilized by an outer pilot. The incoming streams of both the main and pilot jets have the same composition. The main jet nozzle diameter (D) is 12 mm. The pilot stream is supplied through a perforated plate (1175 holes of 1 mm in diameter) around the main jet, with an outer diameter of 5.67D. The Reynolds numbers used in the present work are Re=24,000 (flame F3) and Re=52,000 (flame F1). Based on the estimated characteristic length and time scale given in Chen et al. (1996), flame F1 & F3 correspond to the thin reaction zone regime.

The computational domain extends 20D downstream of the fuel-air nozzle exit, 4D upstream of the nozzle exit and 4D in the radial direction as shown in Fig 7.2. Two different LES grids are studied (for cold flow only): one that consists of 300x94x64 grid points downstream of the nozzle exit plus 50x21x64 grid points upstream, and corresponds to approximately 1.88M grid points (mesh1: coarse). The finer mesh consists of 444x140x96 grid points downstream of the nozzle plus 74x31x96 grid points upstream, and contains approximately 5.91M grid points (mesh2: fine). More close-up view of the computational grid with 1.88M grid points is shown in Fig 7.3. The grid resolution in the computational domain with 1.88M grid points (Fig 7.3) is
Figure 7.1: Schematic diagram of the Bunsen Burner [Chen et al., 1996]

Figure 7.2: A schematic of Bunsen burner: premixed flame configuration.
Figure 7.3: Close-up view of the computational grid
given as: (a) $\Delta x=0.08$ mm is maintained throughout the whole domain starting from jet inlet to outlet, (b) along the central jet $\Delta r=0.047$ mm and $\Delta \theta=0.05$ mm is maintained, (c) in the shear layer $\Delta r=0.047$ mm and $\Delta \theta=0.17$ is maintained, and (d) finally at the lateral boundary $\Delta r=0.06$ mm and $\Delta \theta=0.47$ mm is maintained. More detailed results of the grid independence study are presented in (De & Acharya, 2009).

At the inflow boundary, the instantaneous velocities are computed using two different procedures: (a) experimental data base, and (b) random flow generation technique (Smirnov et al., 2001). Convective boundary conditions (Akselvoll et al., 1996) are prescribed at the outflow boundary, and stress-free conditions are applied on the lateral boundary in order to allow the entrainment of fluid into domain. The time step used for the computation is $dt=1.0e-3$, and the heated pilot temperature is chosen 2005K. The inlet temperature of the main premixed fuel-air jet and the initial temperature in the calculation domain is specified as 300K.

7.2 Chemistry Model

As all the species are explicitly resolved on the computational grid, the Thickened Flame model is best suited to resolve major species. Intermediate radicals with very short time scales (compared to flow motions) are computationally difficult to resolve since such resolution may induce a prohibitive thickening to major species. To resolve intermediate radicals may need a substantially larger computational grid. Therefore from the perspective of balancing accuracy and computational economy, 1 ans 2 step reaction chemistry are explored in the present work.

A single step scheme, which includes five species (CH$_4$,O$_2$,H$_2$O,CO$_2$ and N$_2$) is given by the following expression.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \quad (7.1)$$

where the reaction rate expression is given by

$$q_1 = Aexp(-T_a/T)[CH_4]^a[O_2]^b \quad (7.2)$$
The activation temperature $T_a$ is 24,358 K, parameters $a=0.2$, $b=1.3$, and preexponential factor $A=2.29\times10^{13}$ as given Kim et al. (2006).

A two step chemistry, which includes six species (CH$_4$,O$_2$,H$_2$O,CO$_2$,CO and N$_2$) is given by the following equation set.

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$$  \hspace{1cm} (7.3)

$$CO + 0.5O_2 \leftrightarrow CO_2$$

The corresponding reaction rate expressions are given by:

$$q_1 = A_1 e^{(-E_a^1/RT)}[CH_4]^{a_1}[O_2]^{b_1}$$  \hspace{1cm} (7.4)

$$q_2(f) = A_2 e^{(-E_a^2/RT)}[CO][O_2]^{b_2}$$

$$q_2(b) = A_2 e^{(-E_a^2/RT)}[CO_2]$$

where the activation energy $E_a^1=34500$ cal/mol, $E_a^2=12000$ cal/mol, $a_1=0.9$, $b_1=1.1$, $b_2=0.5$, and $A_1$ and $A_2$ are $2.6\times10^5$ and $1.6\times10^5$, respectively, as given by Selle et al. (2004). Properties including density of mixtures are calculated using CHEMKIN-II (Kee et al., 1989) and TRANFIT (Kee et al., 1986) depending on the local temperature and the composition of the mixtures at 1 atm. In the literature by Selle et al. (2004), they have compared this two-step scheme with GRI mechanism and showed that this two-step mechanism yields fairly good comparison with respect to measured temperatures, burnt gas temperatures, major species mass fractions and flame speeds for a range of fuel-air ratios.

7.3 Non Reacting Flow Results: $Re=24000$

In order to validate the flow solver, LES calculation for the non-reacting flow is reported in this section for $Re=24000$. That ensures that the grid and boundary conditions are properly chosen, and that the subgrid model is able to capture the modeled turbulence adequately.

Figure 7.4 represents the instantaneous snap shot of the velocity fields. The evolution of three components of velocities is clearly observed and shows that the radial and tangential velocities
are of the same order of magnitude, and considerably lower in magnitude relative to the peak axial velocity. The premixed-jet breakup appears to occur about 3-4 jet-diameters downstream of injection.

7.3.1 Mean Axial Velocity

The mean axial velocity profiles in the radial directions at different axial locations are shown in Fig. 7.5. The time-averaged mean velocity is normalized by the bulk velocity \( U_o = 30 \text{ m/s} \). As observed from the experimental data and predictions, the jet shows the expected spreading behavior. The potential core appears to persist up to about \( X/D = 4.5 \), beyond which the centerline mean velocity decreases as the jet expands in the radial direction. These effects are well reproduced by the LES simulations, and the overall predictions are in good agreement with the experimental results. Moreover, the coarse mesh (1.88M grid points) results are in good agreement with the fine mesh (5.91M grid points), and indicate that the 1.88M node calculations are grid-independent.

7.3.2 Turbulent Kinetic Energy

The radial profile of the turbulent kinetic energy, normalized by square of the bulk velocity, at different axial locations is shown in Fig. 7.6. It is evident from the figure that the computed results are reasonably well predicted and compare well with the experimental data set. At \( X/D = 4.5 \), the center line peak value for the fine mesh is slightly over predicted, but at \( X/D = 6.5 \) this over-prediction is eliminated. The evolution of kinetic energy follows the expected trend and initially shows the kinetic energy peak in the mixing layer formed by the primary-jet and the coaxial air-stream. Further downstream, the mixing layers merge and the kinetic energy peak moves toward the centerline as seen at \( X/D = 8.5 \).

7.4 Reacting Flow Results: TF Model for \( \text{Re}=24000 \)

Figure 7.7 shows a typical evolution of instantaneous flame front, which is represented by the temperature field. As time increases the flame front is seen to expand radially and in the
downstream directions with the burnt regions having higher flame temperatures, and the unburnt regions (in blue) at lower temperatures. The cusp formation (regions with negative curvature) is clearly observed from the instantaneous field along the boundaries of the burnt (product side) and unburnt (air or premixed fuel-air side) regions. The cusps are usually formed towards the product side, where the flow field is accelerated due to the heat release from the flame. However, the small scale cusp formation is reduced by thickening the flame front artificially (seen as narrow band in Fig 7.7), and this reduces the flame wrinkling as well.

7.4.1 Comparison of TF Model and its Variants

In this section, the comparison of different TF model and its variants are reported in the context of 2-step and 1-step chemistry. The instantaneous inflow boundary conditions for all of these calculations are prescribed using the experimental date base. The time step used for the computation is $dt=1.0e-3$, and the heated pilot temperature is chosen 2005K. The inlet temperature of the main premixed fuel-air jet and the initial temperature in the calculation domain is specified as 300K.

7.4.1.1 Mean Axial Velocity

Figure 7.8 and Figure 7.9 shows the mean axial velocity profiles at different axial locations obtained using 2-step and 1-step global chemistry, respectively. Also shown are the predictions of Lindstedt et al. (2005) (used PDF model for his calculations) and Duchamp et al. (2002) (used G-equation for his simulations). Figures 7.8-7.9 show that the overall velocity predictions using different variants of the thickened-flame models with both singe-step and two-step chemistry are in reasonably good agreement with experimental data and the PDF model predictions except at the two downstream locations of $X/D=6.5$ and $X/D=8.5$, where the predicted spreading rate is not in agreement with the data (predictions show higher spreading along the inner edge of the mixing layer). These discrepancies are linked to higher kinetic energy predictions in the mixing layer region. The PDF model predictions are comparable with the thickened flame model predictions at
X/D=2.5 and 4.5, but show better agreement with the data at X/D=6.5 and 8.5, while G-equation model consistently overpredicts at the first three locations (X/D=2.5, X/D=4.5, and X/D=6.5).

The single-step power-law thickened flame model appears to have the best agreement with the mean velocity data and the PDF model. This appears to be a fortuitous result since one would expect the two-step chemistry model to show better agreement.

7.4.1.2 Turbulent Kinetic Energy

Turbulent kinetic energy predictions using the different thickened flame models are shown in Figures 7.10 and 7.11. The discrepancies are clearly observed close to the nozzle exit where the thickened flame models underpredict the turbulence levels in the vicinity of the centerline at axial locations X/D=2.5 and X/D=4.5. The peak values along the shear layer are in better agreement in the near-field of injection, but further downstream overpredict the turbulence in the mixing layer and flame regions. The power-law and the dynamically-thickened flame models appear to improve the model predictions downstream (X/D=8.5) where the baseline thickened flame model overpredicts the centerline values. The PDF model overpredicts the turbulence levels at all radial locations in the near-field of injection, but appear to be in qualitatively good agreement with the power law and the dynamically thickened model predictions at X/D=6.5 and 8.5. The G-equation model overpredicts all the locations excluding X/D=2.5, and generally shows the poorest performance.

In comparing the 1-step and 2-step chemistry models, it is observed that the 1-step power-law model predictions are in reasonable and better agreement with the PDF model predictions. This explains the improved mean velocity predictions with the 1-step power law model compared to the other models.

7.4.1.3 Mean Temperature

Mean temperature profiles obtained from different chemistry models are presented in Figs. 7.12-7.13. The mean progress variable is defined as \( C = (T-T_{u})/(T_b-T_{u}) \), where \( T_u = 298K \) and
$T_b = 2248$ K.

Immediately downstream of the nozzle exit ($X/D = 2.5$), the temperature is over-predicted due to the effect of chosen pilot boundary conditions as well as heat loses from the burner surface. However, further downstream ($X/D = 4.5$, $X/D = 6.5$) the predictions are in better agreement with the data. In particular the power-law and the PDF models show good agreement, while the G-equation consistently shows an over prediction. At $X/D = 8.5$ all models, excluding G-equation, under-predict the measured temperature distribution. It is apparent that the spreading of the temperature shear layer is not being correctly predicted by all models.

In examining the single-step chemistry model predictions, it is clear that all variants of TF models underpredict the temperature distributions and the width of the temperature shear layer. Clearly, the one step global chemistry does not reproduce the mean temperature properly; however it provides useful qualitative information. The baseline thickened flame model predictions are clearly improved by the power-law and the dynamically thickened-flame models. The mean reaction rate in the governing equation, which is modified by the thickening factor and efficiency function, is always under-estimated in the baseline thickened flame model to a greater extent than that in the power law model. This produces lower reaction rates in the baseline model and leads to lower prediction of temperature profiles in the baseline thickened flame model.

### 7.4.1.4 RMS of Reaction Progress Variable

The RMS of reaction progress variables is defined as $C^* = \sqrt{\langle T^* \rangle}/(T_b - T_u)$.

Figures 7.14-7.15 show the RMS of reaction progress variable predictions for 2-step and 1-step chemistry models, respectively. The two-step model predictions show the correct qualitative trends at most locations but generally tend to under-predict the measured values. The single-step predictions are clearly off and do not even produce the right trends of the peak values occurring in the mixing layer region.
7.4.1.5  Turbulent Flame-brush Thickness

The turbulent flame-brush thickness, which is a characteristic representation of the transition zone between burnt and unburnt gases in premixed flames, is computed as

\[ l_{F,t} = \left[ \frac{\partial C}{\partial r} \right]_{\text{max}}^{-1} \quad (7.5) \]

Figure 7.16 shows the comparison of computed flame-brush thickness for all models including experimental data. Each individual section [Fig 7.16(a)-(d)] represents a specific model, for one and two step chemistry, comparison with respect to experiments and other simulations. For 1-step chemistry, all the models over-predict the thickness, while 2 step chemistry shows better predictions. Over-prediction of flame-brush thickness inherently explains the under-prediction of mean reaction progress variable C, which is evident from Figures 7.12-7.13. Among all the models, PDF simulations and 2 step chemistry calculations are in better agreement.

7.4.1.6  Remarks

It is observed that the various TF model predictions do not show any major differences. The dynamic versions of the models do show some improvements, while the power-law model for the two-step chemistry model also shows an improvement in the prediction of the peak kinetic energy. However, the profiles with all the models are relatively close to each other and no one model consistently shows improved prediction over the others at the various X/D locations. Hence, based on this comparison, the original TF model would be an appropriate choice, and therefore, further calculations reported are based on the original TF model. It is also observed that the velocity predictions using the G-eqn. model do not show good agreement with the measurements while both the TF model and the PDF model predictions are in good agreement with the mean velocity data. The turbulent kinetic energy predictions with the PDF model appear to be over-predicted at X/D=2.5 at all radial locations, while the TF model tends to under-predict at radial locations close to centerline.
Regarding different chemistry model comparison, it is also observed that the 2-step chemistry predictions appear to be a significant improvement over 1-step chemistry predictions and agree better with experimental data. Moreover, the different variants of the TF model with 2-step chemistry produce very comparable predictions. Hence, from this point original TF model predictions using 2-step chemistry will be presented. It should be noted that the G-equation model predictions generally over-predict the temperature values significantly and appear to perform much worse than the PDF or TF models.

7.4.2 Original TF Model Results-Deatiled Distributions

Based on the observations so far that show improvements with the two-step chemistry calculations, and no clear difference between the variants of the TF models, additional results will be presented only with the original TF model and with the two-step chemistry calculations. In this section, attention will be focused on detailed comparisons of the TF model, the PDF model, the G-equation model and the experimental data for the mean velocity, temperature, kinetic energy and all major species. This comparison will be presented at several X/D locations (2.5, 4.5, 6.5, and 8.5). The instantaneous velocity at the inflow boundary for these calculations is prescribed using the random inflow generation technique (Smirnov et al., 2001). The time step used for the computation is \( dt=1.0e-3 \), and the heated pilot temperature is chosen 2005K. The inlet temperature of the main premixed fuel-air jet and the initial temperature in the calculation domain is specified as 300K.

7.4.2.1 Mean Axial Velocity

Figure 7.17 shows the mean axial velocity profiles at different axial locations obtained using 2-step global chemistry. Also shown are the predictions of Lindstedt et al. (2005) (used PDF model for his calculations) and Duchamp et al. (2002) (used G-equation for his simulations).

In evaluating the models, the perspective of computational economy must be kept in mind. A multi step calculation require sthe calculation of transport equations for multiple species, and
with a PDF modeling approach, the reaction rate expressions require the use of a look-up table with substantial computational input/output (I/O) requirements. In the Thickened Flame modeling approach, the reaction rate expressions are computed using Arrhenius law, and computational effort including I/O time is expected to be less. However, we have not undertaken a direct study of the two approaches comparing the computational efforts at this stage.

Figure 7.17 shows that the mean velocity predictions using the TF modeling approach and these are in reasonably good agreement with experimental data as well as with the PDF model predictions. At the downstream locations, the TF model predictions show higher spreading along the inner edge of the mixing layer (the PDF model shows a similar behavior also). In comparing the models, the G-eqn shows significant over-prediction with the data for X/D<6.5.

The radial profiles of the mean axial velocity show greater radial broadening compared to the non-reacting case (as shown in Fig. 7.5), due the effect of the flame front, pushing the shear layer outward in the radial direction. Furthermore, it is observed that the peak center line velocity remains almost constant in the axial direction, and exhibits a longer potential core compared to the non-reacting case. These effects are reasonably well reproduced by the simulations.

7.4.2.2 Turbulent Kinetic Energy

Turbulent kinetic energy predictions using the TF modeling approach are shown in Figure 7.18. As it is evident from the experimental data there are significant differences observed while compared to the non-reacting case (Fig. 7.6). The measured turbulent kinetic energy initially increases with axial distance for the reacting case while it decreases for the non-reacting case. Furthermore, for the reacting case, the kinetic energy peak moves away from the centerline (due to radial expansion of the flame front) with increasing axial direction while the peak moves towards centerline in the non-reacting case due to turbulent diffusion effects.

The predicted kinetic energy shows significant differences between the various models. The TF model shows an initial under-prediction close to the centerline (at X/D=2.5), but the peak values
and the general trend is well predicted by the TF model. At the downstream locations (X/D=4.5 and 6.5), the TF model predictions are in reasonably good agreement with the experimental data. The PDF model over predicts the turbulence levels at all radial locations in the near field of injection, but appears to be in better agreement with the measured data at X/D=8.5. The G-equation model generally shows the poorest performance excluding the near-injection location at X/D=2.5 where the agreement is reasonable. These discrepancies are linked with the mean temperature predictions and discussed in the following sub-section. Clearly, in assessing all X/D locations, the TF model predictions appear to provide the best agreement with the data.

7.4.2.3 Mean Temperature

Mean temperature profiles are presented in Figure 7.19. Immediately downstream of the nozzle exit (X/D=2.5), the temperature is over-predicted due to the effect of the 2-step chemistry model (as opposed to more complex chemistry schemes) and is likely to over-predict temperature in fuel-rich regions. However, further downstream (X/D=4.5, X/D=6.5) the peak temperature predictions with the TF model and the PDF models are in better agreement with the data. In particular, the TF model and the PDF model show good agreement, while the G-equation consistently shows an over prediction. At X/D=8.5 all models excluding the G-equation under-predict the measured temperature distribution. With the TF model, it is apparent that the spreading of the temperature shear layer is not being correctly predicted, and that this is likely due to the artificial thickening of the flame front and the scalar diffusivity in the flame region. It can be seen that the centerline mean temperature increases downstream in the experiments, whereas it remains close to the unburnt temperature in the TF simulation. While both the PDF model and the TF model show qualitatively similar behavior, the PDF model does show somewhat better agreement with the temperature data. This is a consequence of the more detailed chemistry calculations incorporated in their models. Despite this, the poorer predictions of the turbulent kinetic energy with the PDF model, relative to the TF model, are puzzling.
7.4.2.4 Species Mass Fraction

The radial distributions of the major species mass fractions are presented in the Figures 7.20 - 7.24. In presenting these results, the G-equation model calculations are not presented here since the detailed data with this model is not available.

Figure 7.20 shows the mean CH$_4$ distributions at the four radial locations. The profile of the curve clearly shows the premixed unburnt core (plateau region near the centerline), the flame region where methane is consumed (represented by the decay region), and the burnt or outer region where no methane is present. It can be seen that only by X/D=8.5 does the flame region start approaching the centerline. The TF model predictions are in excellent agreement with the data, and the level of agreement is even better than that observed with the PDF model. The O$_2$ concentrations are shown in Fig. 7.21, exhibit distributions similar to the CH$_4$ curve, and the experimental trends are well captured by both the TF model the PDF model. The TF model appears to over-predict oxygen concentrations in the outer regions. This observation leads to an under-prediction of H$_2$O in the outer regions as well (Fig. 7.24).

CO$_2$ concentrations are also in good agreement with the measurements (Fig. 7.23) at all X/D locations, while CO predictions (Fig. 7.22) show excellent agreement at X/D of 2.5 but under-predict at other X/D locations. This may possibly be due to the lower O$_2$ consumption. However, PDF model simulations always significantly over estimate the CO concentrations, and also underestimate CO$_2$ concentrations. At this stage, the discrepancies in CO predictions are not very clear; hence one needs to be more careful in interpreting the data.

7.4.3 Conclusions

A thickened flame approach is used to compute the piloted premixed stoichiometric methane-air flame for Reynolds number Re = 24,000. The original TF model and its variants including the Power-law flame wrinkling model, and the dynamically modified version of these models in conjunction with two different chemistry models have been implemented and compared. In the
first part of the work, the comparison between various TF models and different chemistry models has been presented.

It has been shown that the various variants of TF model produce close agreement with each other using 2-step chemistry model. However, they do exhibit some differences while using 1-step chemistry. Moreover, the 2-step chemistry model appears to perform better over 1-step chemistry model. In the second part of the work the detailed results using the original TF model with 2-step chemistry have been reported.

The original TF model predictions with 2-step chemistry have been found to be in satisfactory agreement with the experimental data and with the more detailed PDF simulations. The mean reaction progress variable and the mean axial velocity are well predicted in the near-field while showing some discrepancies at the downstream locations. The turbulent kinetic energy is under-predicted in the vicinity of the centerline at axial locations X/D=2.5, but matches well at the locations X/D=4.5-8.5. The major species mass fraction predictions are also in good agreement with the exception of CO that is under-predicted by the TF model and over-predicted by the PDF model. In general, the TF model and the previously published PDF model predictions are in reasonable agreement with each other and experiments, whereas the G-equation model predictions show poor performance.

In comparing the computational resources, the TF model is always been less computationally expensive compared to PDF model where the use of a look-up table takes substantial computational input/output (I/O) requirements. However, TF model simulations at this stage are restricted to very few number of chemical kinetics (1 or 2-step chemistry) while producing reasonably good agreement of the data.
Figure 7.4: Instantaneous snap shots of the velocity field (m/s) for Re=24000
Figure 7.5: Cold flow (Re=24000): mean axial velocity $U/U_0$. Experimental data is shown by symbols (Δ) and lines are LES results: solid lines (—, mesh1: coarse), dashed lines (- - -, mesh2: fine)
Figure 7.6: Cold flow (Re=2400): TKE ($k/U_o^2$). Legend—See Fig. 7.5
Figure 7.7: Instantaneous flame front (temperature in K scale) for Re=24000
Figure 7.8: Reacting flow (2 step chemistry, Re=24000): mean axial velocity $U/U_o$. Experimental data ($\Delta$), Lindstedt simulations (●, blue dots), Duchamp simulations (・, green box), TF model (—, solid lines), power law (- - -, dashed lines), dynamically modified TF model (－－－, dashed-dot lines), dynamically modified power law model (－－－－, long-dashed lines)
Figure 7.9: Reacting flow (1 step chemistry, Re=24000): mean axial velocity $U/U_o$. Legend-See Fig. 7.8
Figure 7.10: Reacting flow (2 step chemistry, $Re=24000$): turbulent kinetic energy $k/U_o^2$. Legend—See Fig. 7.8.
Figure 7.11: Reacting flow (1 step chemistry, Re=24000): turbulent kinetic energy $k/U_o^2$. Legend—See Fig. 7.8
Figure 7.12: Reacting flow (2 step chemistry, Re=24000): mean reaction progress variable C. Legend-See Fig. 7.8
Figure 7.13: Reacting flow (1 step chemistry, Re=24000): mean reaction progress variable C. Legend-See Fig. 7.8
Figure 7.14: Reacting flow (2 step chemistry, Re=24000): RMS of mean reaction progress variable C'. Legend-See Fig. 7.8
Figure 7.15: Reacting flow (1 step chemistry, Re=24000): RMS of mean reaction progress variable $C'$. Legend-See Fig. 7.8
Figure 7.16: Turbulent flame-brush thickness $l_{F,t}(Re=2400)$: Experimental data ($\Delta$, solid lines), Lindstedt simulations ($\circ$, dashed lines), Duchamp simulations ($\square$, dashed-dot lines); (a) TF model (1 step: $\nabla$, dashdotdot lines, 2 step: $\diamond$, long-dash lines), (b) power law (1 step: $\nabla$, dashdotdot lines, 2 step: $\diamond$, long-dash lines), (c) dynamically modified TF model (1 step: $\nabla$, dashdotdot lines, 2 step: $\diamond$, long-dash lines), (d) dynamically modified power law model (1 step: $\nabla$, dashdotdot lines, 2 step: $\diamond$, long-dash lines)
Figure 7.17: Reacting flow : mean axial velocity $U/U_o$. Experimental data (∆), Lindstedt simulations (●, blue dots), Duchamp simulations (○, green box), TF model (—, solid lines)
Figure 7.18: Reacting flow (Re=24000) : TKE (k/U_o^2). Legend-See Fig. 7.17
Figure 7.19: Reacting flow (Re=24000) : mean temperature C. Legen-See Fig. 7.17
Figure 7.20: Reacting flow (Re=24000) : Mean CH₄ concentration. Experimental data (∆), Lindstedt simulations (●, blue dots), TF model (—, solid lines)
Figure 7.21: Reacting flow (Re=24000) : O$_2$ concentration. Legend-See Fig. 7.20
Figure 7.22: Reacting flow (Re=24000) : CO concentration. Legend-See Fig. 7.20
Figure 7.23: Reacting flow (Re=24000) : CO$_2$ concentration. Legend-See Fig. 7.20
Figure 7.24: Reacting flow (Re=24000): H$_2$O concentration. Legend-See Fig. 7.20
7.5 Reacting Flow Results: Modified TF Model

A modified Thickened Flame (TF) model based on Large Eddy Simulation (LES) methodology is used to investigate premixed combustion and the model predictions are evaluated by comparing with the pilot premixed stoichiometric methane-air flame data (Chen et al., 1996) for Reynolds numbers Re = 24,000 (flame F3) and Re=52,000 (flame F1). In this work, the TF model is modified and its performance explored for high Reynolds number flames (De and Acharya, 2009). The basic idea of Thickened-Flame approach is that the flame front is artificially thickened to resolve on the computational LES grid while keeping the laminar flame speed (\( s_L \)) constant. The artificially thickening of the flame front is obtained by enhancing the molecular diffusion and decreasing the pre-exponential factor of the Arrhenius law. Since the flame front is artificially thickened, the response of the thickened flame to turbulence is affected and taken care of by incorporating an efficiency function (E) in the governing equations. The efficiency function (E) in the modified TF model is proposed based on the direct numerical simulations (DNS) data set of flame-vortex interactions (Colin et al., 2000). The adopted generic premixed combustion configuration for which experimental data (Chen et al., 1996) and numerical predictions with other approaches (Hermann, 2006; Lindstedt & Vaos, 2006) are available. Both the considered flames (flame F1 and flame F3) fall in the thin reaction zone regime, and hence the thickened flame modeling approach is applicable.

7.5.1 Results and Discussion

In this section we present the predicted simulations from the LES-modified TF model and compare with the measured data by Chen et al. (1996) as well as with the computations reported using RANS based probability distribution function (PDF) modeling approach by Lindstedt et al. (2006) and RANS based G-equation approach by Hermann (2006). In evaluating the models, the perspective of computational economy must be kept in mind. A multi step calculation requires the calculation of transport equations for multiple species, and with a PDF modeling
Figure 7.25: Reacting flow: Mean axial velocity $U/U_o$ ($Re=24000$). Experimental data ($\Delta$), modified TF model (—, solid lines), original TF model ( - - -, dashed lines)

Figure 7.26: Reacting flow: Axial velocity $U/U_o$ ($Re=52000$). Legend—See Fig. 7.25
approach; the reaction rate expressions require the use of a look-up table with substantial computational input/output (I/O) requirements. In the Thickened Flame modeling approach, the reaction rate expressions are computed using Arrhenius law, and hence computational effort including I/O time is minimized. In terms of CPU costs using TF model, the efficiency for solving 10 PDEs in a fully coupled implicit fashions (reacting flow computations) with 1.88M grid points on a system (15.322 TFlops Peak Performance with 2 Dual-Core 2.66 GHz Intel Xeon 64bit processors and 4 GB RAM per node) is given as: (a) running on 1 processor takes 1703sec/iteration (773.26 microsec/pt/iteration), (b) running on 8 processors takes 48.91sec/iteration (22.21 microsec/pt/iteration), and (c) running on 64 processors takes 8.022sec/iteration (3.64 microsec/pt/iteration).

In presenting the results, we will discuss predictions of the mean axial velocity, turbulent kinetic energy, mean temperature, and species mass fraction. In the first part of this section, we will first examine the sensitivity of the predictions to the choice of two global parameters: the thickening factor F and the pilot temperature. This will be followed by the results from the detailed simulations for low and high Reynolds numbers.

7.5.1.1 Comparison of Original TF Model and Modified TF Model

The original TF formulation is based on the C_n function, Eq. (4.32), as given by Colin et al. (2000). And the modified TF formulation is based on the proposed C_n function, Eq. (4.33). Figures 7.25 - 7.26 show the comparison of the predicted results using two different TF model formulations for flame F1 & F3. Both the TF models produce very comparable predictions, but with some modest improvements with the TF Model proposed in this paper. For flame F3, it is clearly observed that original TF model under-predicts the mean axial velocity in the shear layer region and show greater radial spreading at the downstream locations. For flame F1, the under-prediction by the original TF model is also visible, but greater in magnitude at the location X/D=8.5, as shown in Fig. 7.26.
Figure 7.27: Reacting flow: Mean axial velocity $U/U_o$, turbulent kinetic energy $k/U_o^2$, Mean CH$_4$ concentrations, Mean CO$_2$ concentrations using different thickening factor $F$ (Re=24000). Experimental data ($\Delta$), $F=10$ (---, solid lines), $F=20$ (- - -, dashed lines)

Figure 7.28: Reacting flow: Mean axial velocity $U/U_o$, turbulent kinetic energy $k/U_o^2$, Mean temperature $C$, Mean CH$_4$ concentrations, Mean CO$_2$ concentrations using different pilot temperature (Re=52000). Experimental data ($\Delta$, $\circ$), 2005K (---, solid lines), 1785K (- - -, dashed lines)
Figure 7.29: Reacting flow: Mean axial velocity $U/U_0$ (Re=24000). Experimental data ($\Delta$), Lindstedt simulations with RANS based PDF model (●, blue dots), Hermann simulations with RANS based G eqn. model (●, green squares), Duchamp simulations with LES based G eqn. model (▼, black gradients), TF model (—, solid lines)
Figure 7.30: Reacting flow: Axial velocity $U/U_o$ (Re=52000). Legend—See Fig. 7.29
Figure 7.31: Reacting flow: TKE $k/U_0^2$ (Re=24000). Legend-See Fig. 7.29
Figure 7.32: Reacting flow: TKE $k/U_0^2$ (Re=52000). Legend-See Fig. 7.29
Figure 7.33: Reacting flow: Mean temperature $C$ (Re=24000). Legend-See Fig. 7.29
Figure 7.34: Reacting flow: Mean temperature $C$ (Re=52000). Legend—See Fig. 7.29
Figure 7.35: Reacting flow: CH$_4$ concentrations (Re=24000). Legend-See Fig. 7.29
Figure 7.36: Reacting flow: CH₄ concentrations (Re=52000). Legend-See Fig. 7.29
Figure 7.37: Reacting flow: O$_2$ concentrations (Re=24000). Legend-See Fig. 7.29
Figure 7.38: Reacting flow: O$_2$ concentrations (Re=52000). Legend-See Fig. 7.29
Figure 7.39: Reacting flow: CO₂ concentrations (Re=24000). Legend-See Fig. 7.29
Figure 7.40: Reacting flow: CO₂ concentrations (Re=52000). Legend—See Fig. 7.29
Figure 7.41: Reacting flow: CO concentrations (Re=24000). Legend-See Fig. 7.29
Figure 7.42: Reacting flow: CO concentrations (Re=52000). Legend-See Fig. 7.29
Figure 7.43: Reacting flow: H₂O concentrations (Re=24000). Legend-See Fig. 7.29
Figure 7.44: Reacting flow: H₂O concentrations (Re=52000). Legend-See Fig. 7.29
7.5.1.2 Effects of Thickening Factor (Re=24000)

Figure 7.27 shows the predicted results using two different thickening factors $F$ (=10 and 20) for flame F3 (Re=24000). The thickening factor is a parameter in the TF model that modifies the mean reaction rate and the diffusion terms in the governing equations. However, increasing the thickening factor reduces the Damköhler number, and thus the flow field becomes less sensitive to the turbulence motion. It is observed that the two different thickening factors do not show any major differences in predictions except for the turbulent kinetic energy predictions (Fig 7.27) at the location X/D=6.5 where it is slightly over-predicted with the higher $F$. The kinetic energy predictions show good agreement with data at $F=10$. As expected, as the thickening factor is increased, the reaction rate is decreased and in turn reduces the mean temperatures. As the temperature levels go down, it reduces the local viscosity and increases the kinetic energy predictions. While no specific choices for thickening factor have been proposed in the literature, it has been suggested that the effect of thickening factor becomes significant for the values larger than $F=10$ (Colin et al., 2000). Hence, based on the comparisons made here, the thickening factor $F=10$ would be an appropriate choice, and therefore, further calculations reported are based on the thickening factor $F=10$.

7.5.1.3 Effects of Pilot Temperature (Re=52000)

The effects of different pilot temperatures have been studied and reported in the Figure 7.28 for flame F1 (Re=52000). The mean progress variable is defined as $C=(T-T_u)/(T_b-T_u)$, where the un-burnt temperature $T_u=298$ K and the burnt temperature $T_b=2248$ K. The figure includes the comparison between two different temperature boundary conditions for the heated pilot: one is 2005 K and the other one is 1785 K. No specific pilot temperature data is prescribed in the measurements which can be used as boundary condition for computations. Therefore, the pilot composition was computed based on chemical equilibrium where the enthalpies are taken for 10% and 20% heat loses to burner, corresponding to pilot temperatures are 2005 and 1785K (Lindstedt
& Vaos, 2006). It is clearly observed that the different pilot temperature boundary conditions produce very comparable predictions except for the predicted temperature in the flame region which is slightly lower in the case of lower pilot temperature, i.e. 1785 K. Hence, from this point we will present predictions using the pilot temperature boundary condition as 2005 K.

7.5.1.4 Modified TF Model Results-Detailed Distributions

Based on the observations so far, additional results will be presented with the modified TF model using the thickening factor F=10 and pilot temperature boundary condition as 2005 K. In this section, attention will be focused on detailed comparisons of the modified TF model, the RANS based PDF and the G-equation model and the experimental data for the mean velocity, temperature, kinetic energy and all major species. This comparison will be presented at several X/D locations (2.5, 4.5, 6.5, and 8.5).

It should be noted that the present LES simulations are compared with published simulations from other RANS based model predictions with the PDF approach (Lindstedt and Vaos, 2006) and G-equation approach (Hermann, 2006) for the same flame data at the two Reynolds numbers (24,000 and 52,000). At the lower Re, LES predictions with the G-equation approach (Duchamp and Pitsch, 2000) are also available, and we have also included this in the comparison. However it should be noted that the various simulations presented use different numerics and chemistry compared to the present simulations. Therefore, a one-to-one comparison is not possible between all these models, and the performance of the various models should be viewed from this perspective.

Mean Axial Velocity Figures 7.29 & 7.30 show the mean axial velocity profiles at different axial locations for Re=24000 (flame F3) and Re=52000 (flame F1), respectively. The overall velocity predictions using modified Thickened Flame model are in reasonably good agreement with experimental data as well as with the PDF model predictions. At the lower Re, the TF model
predictions show a slightly greater spreading in the mixing layer. At the higher Re, both the TF and PDF model predictions are in excellent agreement with the measurements. The RANS based G-eqn model shows over-predictions particularly for the lower Reynolds number case. Similar trends are also observed with the LES based G-eqn simulations as reported by Duchamp et al. (2000).

When compared with cold flow predictions (Fig. 7.5), the radial profiles of the mean axial velocity are broadened in the reacting case, due the effect of the flame front, pushing the shear layer outward in the radial direction. Furthermore, it is observed that the peak center line velocity remains almost constant in the axial direction, and exhibits a longer potential core compared to the cold flow case. These effects are reasonably well reproduced by the present simulations.

**Turbulent Kinetic Energy** Turbulent kinetic energy predictions for the reacting flow using the modified TF model are shown in Figures 7.31 and 7.32. In general, the agreement between the measured and predicted kinetic energy profiles is excellent. It is observed that the measured and predicted turbulent kinetic energy along the centerline increase at the downstream for the non-reacting case (Fig. 7.6) while it remains almost constant for the reacting case. Also, the peak value of kinetic energy decreases in the axial direction for the non-reacting case, whereas it increases for the reacting case. Furthermore, for the reacting case, the kinetic energy peak moves away from the centerline further downstream (as the jet entrains air), while it moves towards the centerline for the non-reacting case (Fig. 7.6).

The kinetic energy simulations for the reacting flow clearly show differences compared to the measured data. For flame F3 (Re=24000), the general trends are well predicted with the TF model till about X/D=6.5. The PDF model consistently shows over-prediction of the turbulence levels at all radial locations and particularly upto X/D=6.5. The RANS-based G-equation model shows reasonable agreement till X/D=4.5 and then shows under-prediction at the downstream
locations (X/D=6.5 and X/D=8.5) for r/D>0.5. However, it should be noted that the LES coupled G-eqn simulation (Duchamp & Pitsch, 2000) shows over-predictions in the kinetic energy at all the locations excluding X/D=2.5 where it shows better agreement. The differences in the kinetic energy predictions between the LES results in (Duchamp & Pitsch, 2000) and the RANS results in (Hermann, 2006) are presumably linked to the turbulence modeling issue.

At the higher Reynolds number, for flame F1 (Re=52000), the present simulations are in good agreement with data and capture the general trend quite well, even at the downstream location of X/D=8.5 where, at the lower Re, the TF model under-predicted the measurements. At the location X/D=2.5, close to nozzle exit, the modified TF model under-predicts the turbulence levels in the inner edge of shear layer; however, the model predictions appear to improve at the downstream locations (X/D=4.5, 6.5 and 8.5) where the general trends and peak values are well predicted. In comparing the different model predictions, the TF and PDF model predictions show good agreement with the data while the RANS based G-eqn model under-predicts the peak values by 35-50% at the downstream locations of X/D=6.5 & 8.5. These discrepancies are explained using the mean temperature predictions and discussed in the following sub-section. As observed clearly, in assessing different model predictions, both the modified TF model and PDF model predictions appear to provide reasonably good agreement with the data.

Comparing the TF model predictions at different Reynolds numbers, it is evident that the modified TF model appears to improve the results at the higher Reynolds number. This means the efficiency function parameter E in the governing Eqn. (12) is better suited to properly estimate the flame-turbulence interaction at higher turbulence intensity. This issue of accurately parametrizing the efficiency function needs more investigation.

**Mean Temperature**  Mean temperature profiles obtained for different Reynolds numbers are presented in Figs. 7.33 and 7.34. The mean progress variable is defined as \( C = (T-T_u)/(T_b-T_u) \),
where $T_u = 298$ K and $T_b = 2248$ K. It is immediately evident from the measured temperature distributions at the two Reynolds numbers that the maximum temperature is reduced as the jet velocity (Reynolds number) is increased. This fact can be explained by the fact that as the jet velocity increases, more cold ambient air is entrained on the bunt side of the flame, thus reducing the maximum temperature. This behavior is seen consistently in both the data and the model predictions.

For flame F3 (Re=24000, Fig. 7.33), as observed immediately downstream of the nozzle exit (X/D=2.5), the mean temperature profile shows an over-prediction. This is likely due to the effect of the chosen 2-step chemistry model, which is based on a reduced complex chemistry and very much likely to over-predict temperature in the fuel-rich regions. However, at the downstream locations (X/D=4.5, 6.5 and 8.5) the mean temperature predictions are in better agreement with the data. In particular, both the modified TF model and the PDF model predictions show good agreement, while both the RANS and LES based G-equation simulations consistently show an over prediction. At all the X/D locations, the G-eqn temperature predictions exhibit a radial shift of the shear layer towards the centerline. One deficiency in the TF model predictions at the lower Re is that the spreading of the temperature shear layer is under-estimated, and this is most likely due to the artificial thickening of the flame front and the diffusivity in the shear layer. Also, it is noticed that the downstream centerline mean temperature in all the simulations excluding LES based G-eqn simulation remains almost close to the un-burnt temperature, whereas it increases in the experiment. For the TF model, this may be linked to the under-prediction of the kinetic energy (and the turbulent diffusivity) near the centerline observed in Fig. 7.31.

In Figure 7.34 for flame F1 (Re=52000), there is a greater over prediction of the maximum temperature by the modified TF model at X/D=2.5; further downstream, for higher values of X/D the mean temperature profile is captured very well. Comparing all the model predictions, the PDF
model consistently shows over-predictions at all the axial locations, whereas the RANS based
G-eqn model shows overall better agreement with the data excluding the locations X/D=2.5 &
4.5 where it shows under-prediction of the maximum temperature. The over-prediction by the
modified TF model in the near-field, as noted earlier, is possibly due to the chosen chemistry
scheme, which is likely to produce higher flame temperature in the fuel rich regions (close to
the nozzle exit). Surprisingly, the PDF model predictions consistently show high temperature
distributions in spite of using more detailed chemistry calculations in their model and yielding
reasonably good turbulent kinetic energy predictions though (Fig. 7.32). On the other hand, the
RANS based G-eqn shows overall better agreement in predictions of temperature profiles, but as
seen in Fig. 7.32, the turbulent kinetic energy predictions exhibited over-predictions in the near
field and lower peak kinetic energies in the far field.

Comparing different Reynolds numbers, it is clearly observed that the modified TF model
appears to improve the results for higher Reynolds number, capturing both the trends as well
the magnitude of the maximum temperature. As the Reynolds number increases, the maximum
temperature also decreases due to the greater entrainment of cold ambient air driven by the higher
jet velocity. Compared to the lower Reynolds number (Re=24000), where the thermal shear layer
was thinner than in the data, the temperature profile at the downstream location (X/D=8.5) is
properly predicted for the higher Re. This better agreement of the temperature field with the data
at the higher Reynolds number is consistent with similar observations for the mean axial velocity
and turbulent kinetic energy predictions (Figs. 7.30 and 7.32).

Species Mass Fraction The radial distributions of the major species mass fractions are
presented in the Figures 7.35 - 7.44. For flame F3 (Re=24000), mean CH₄ concentrations are
well captured by the modified TF model (Fig. 7.35). The PDF model also shows good agreement
except for a modest over-prediction at the lower Re. However, RANS based G-eqn predictions
show a consistent under-prediction and an apparent discrepancy in the radial mean flame front positions at all the axial locations. This radial shift can be linked with the mean temperature profile (Fig. 7.33) which also shows radial movement towards centerline. The profile of CH₄ curve clearly shows the premixed un-burnt core (plateau region near the centerline), the flame region where methane is consumed (represented by the decay region), and the burnt or outer region where no methane is present. In general, the modified TF model predictions are in excellent agreement with the data, and the level of agreement is even better than that observed with the PDF model. The O₂ concentrations are shown in Fig. 7.37, exhibit distributions similar to the CH₄ curve, and the experimental trends are well captured by both the modified TF model the PDF model; however, the G-eqn predictions show similar trends of radial shift in the flame region. The modified TF model appears to over-predict oxygen concentrations in the outer regions. This observation leads to an under-prediction of H₂O in the outer regions as well (Fig. 7.43). CO₂ concentrations with the TF model are also in good agreement with the measurements (Fig. 7.39) at all X/D locations, and in fact show better agreement compared to other simulations. CO predictions (Fig. 7.41) show excellent agreement at X/D of 2.5 but under-predict at other X/D locations. This may possibly be due to the lower O₂ consumption. However, both the RANS based model simulations, i.e. PDF model and G-eqn model, always significantly over estimate the CO concentrations.

In the case of flame F1 (Re=52000), mean CH₄ concentrations are well reproduced by modified TF model (Fig. 7.36) and show predictions that are similar to the case of flame F3. However, O₂ concentrations (Fig. 7.38) show under predictions at the downstream locations and correlate with the slight over-prediction of CH₄. This is happening due to enhanced mixing with cold ambient air which is entrained to a greater extent due to the higher jet velocity, and reduces the O₂ consumption. As a consequence, CO₂ and H₂O productions also go down as shown in Figs.
7.40 & 7.44. Mean CO concentrations are also under predicted in this case (Fig. 7.42) as at the lower Re. Comparing the results of all the simulations, the modified TF model shows overall good agreement with the data, whereas both the RANS based models (PDF and G-eqn model) consistently overestimate the CO concentrations and underestimate the CO₂ production.

7.5.2 Conclusions

In this work, a modified Thickened Flame model is used to compute the piloted premixed stoichiometric methane-air flame for the Reynolds number Re = 24,000 and 52,000. Detailed results using the modified TF model with thickening factor of 10 (F=10) and pilot temperature of 2005 K have been obtained with a 2-step chemistry model. These results have been compared with the measurements as well as with other RANS based simulation results using a PDF model and a G-equation model.

The modified TF model predictions with 2-step chemistry have been found to be in satisfactory agreement with the experimental data. The mean axial velocity is well predicted for both the flames, i.e. flame F3 (Re=24000) and flame F1 (Re=52000), but shows higher spreading rate at the downstream locations, especially for low Reynolds number case. In the flame region for flame F3 (Re=24000), the mean reaction progress variable appears to be under predicted along the inner flame brush region, but matches well with the data in the case of flame F1 (Re=52000). The turbulent kinetic energy is under-predicted in the vicinity of the centerline in the near field of injection for both the flames, but is generally well captured at the downstream locations. The major species mass fraction predictions are also in good agreement for both the flames, excluding the CO prediction that is consistently under-predicted.

In general, the modified TF model predictions appear to be in reasonable agreement with the data and show improvement in results in the case of high Reynolds number. The RANS based PDF model simulations generally are in reasonable agreement with the data and the TF model except for an over-prediction of the kinetic energy at the lower Re and a significant over-estimation of the
CO levels. The other RANS based approach, G-eqn. model predictions, are usually not in good agreement with the data; they show a radial-shift of the flame brush region, an over-estimation of the progress variable and CO at the lower Reynolds number. Moreover, the LES coupled G-eqn predictions also do not show good agreement with the data, especially for the lower Re.

In comparing the computational resources, the modified TF model is less computationally expensive compared to PDF model where the use of a look-up table takes substantial computational input/output (I/O) requirements. However, the modified TF model simulations at this stage are restricted to very few number of chemical kinetics (1 or 2-step chemistry), but the present simulations demonstrate reasonably good agreement with the data.
Chapter 8 Natural Gas Combustion in an Unconfined Swirl Stabilized Burner *

An unconfined strongly swirled flow is investigated for different Reynolds numbers using particle image velocimetry (PIV) and Large Eddy Simulation (LES) with a Thickened Flame (TF) model. Both reacting and non-reacting flow results are presented (De et al., 2009). This swirl stabilized burner is of great interest in Land-based gas turbine applications. Land-based gas turbines operate primarily in a lean premixed mode (LPM) with natural gas as the fuel of choice due, in part, to environmental regulations of reducing NOx. LPM combustors operate close to the lean blow out limit and are characterized by low emissions. Swirl is used to provide flame-holding, and plays an important role in these low-NOx gas turbine combustors (Lefebvre, 1999; Syred et al., 1974). In premixed flames, several previous studies have been reported experimentally that characterize the flame structure and provide insight into the flame-turbulence interaction in laboratory scale burners (Cheng, 2000; Schneider et al., 2005; Al-Abdeli and Masri, 2007). Since experiments are generally expensive to undertake, in order to properly design premixed combustion systems, accurate predictions of premixed flames are desirable. Since the capability of the classical approach using Reynolds averaged Navier-Stokes (RANS) equations in conjunction with phenomenological combustion models (Poisnot and Veynante, 2001) is limited, numerical simulations of reacting flows based on large eddy simulations (LES) are well suited to provide accurate and cost-effective predictions. The main philosophy behind LES of a reacting flow is to explicitly simulate the large scales of the flow and reactions, and to model the small scales. Hence, it is capable of capturing the unsteady phenomenon more accurately. The unresolved small scales or sub-grid scales must be modeled accurately to include the interaction between the turbulent scales. Since the typical premixed flame thickness is smaller than the

* Portions of this chapter have appeared in the literature: GT2009-60230.
computational grid (Δ), the small scale or sub-grid scale modeling must also take care of the interaction between turbulence and the combustion processes. In the LES-TF approach, the flame is artificially thickened to resolve it on computational grid points where reaction rates from kinetic models are specified using reduced mechanisms. The influence of turbulence is represented by a parameterized efficiency function. A key advantage of the TF model is that it directly solves the species transport equations and uses the Arrhenius formulation for the evaluation of the reaction rates.

Figure 8.1: Schematic view of the experimental setup

The configuration of interest in the present work is that of a swirl-stabilized flame. An extensive review on swirling flows can be found in (Schneider et al., 2005; Syred et al., 1974; Lucca-Negro et al., 2001). Chanaud (1965), in his pioneering study, reported periodic vortex instabilities in a certain regime of Reynolds number and swirl numbers. These were identified to be the precision vortex core (PVC). Tangirala et al. (1987) studied a non-premixed swirl burner where they reported that the mixing and flame stability can be improved with swirl upto a swirl
number of about unity, beyond which a further increase in swirl reduces the turbulence level as well as the flame stability. Broda et al. (1998) and Seo (1999) experimentally investigated the combustion dynamics in a lean-premixed swirl stabilized combustor. One of the key influences of the swirl on the flow field is the formation of the recirculation zone at the burner exit. As the swirl number exceeds a critical value, vortex breakdown takes place and leads to the formation of an internal recirculation zone (Huang and Young, 2005). The shape and size of the recirculation zone largely depends on swirl and Reynolds numbers (Al-abdeli and Masri, 2007). This recirculation not only enhances fuel-air mixing, but also carries hot products back to the reactants and plays an important role in the flame holding. However, despite several years of research, the mechanisms of vortex breakdown are only partially understood (Lucca-Negro et al., 2001; Syred, 2006; Duwig et al., 2007). In general, strongly swirled flows contain large coherent vortex structures that include the precessing vortex core (PVC). The PVC phenomena occurs when the recirculation zone is displaced from the axis of symmetry and can be damped with reactions (Froud et al., 1995). Recently, a number of studies have analyzed swirling flames using either numerical approaches (Freitag and Janicka, 2007) or experimental techniques (Al-abdeli and Masri, 2007; Al-abdeli and Masri, 2004; Wicksall et al., 2005; Tanahashi et al., 2005; Jarvis and Hargrave, 2006; Jun and Gore, 2002; Frank et al., 1999). The numerical approaches have primarily been RANS-based approaches (Pope, 1985) while many of the experimental studies have used particle image velocimetry (PIV) to measure the flow characteristics in flames.

In this investigation, we employ both computational and experimental methods, to investigate premixed swirl-stabilized flames (De et al., 2009). The experimental approach uses particle image velocimetry (PIV) and an intensified CCD imaging of flame CH-chemiluminescence. The computational method invoked here uses LES combined with a TF approach for combustion. A key task is the assessment of LES-TF model predictions through validations with measurements
in this study. A second task is to use the validated model predictions to analyze the flow and combustion physics and, in particular, to explore how increasing flow velocities alter the vortical structures and the associated heat release behavior which play an important role in the flame holding and blow-off behavior.

8.1 Flow Configuration and Experimental Techniques

The configuration considered here is an unconfined swirl burner. The schematic of the experimental setup is shown in Figure 8.1. It includes the combustor, the PIV system for the velocity measurement, and the PI-MAX ICCD camera (Princeton Instruments) for CH-emissions measurement. The combustor consists of the inlet fuel and air-delivery system, and the premixing section. The flame is swirl-stabilized and attached to the center body at the dump plane for conditions corresponding to the measurements in this study.

The 45° swirl vane is fitted with a solid center body which also acts as a fuel injector (Fig. 8.2). This center body extends beyond the swirl vane and is flush with the dump plane of the combustor. The diameter of the center body is 12.7 mm (0.5 inch) and the O.D. of the swirler is 34.9 mm (1.375 inch). Methane gas is injected radially from the center body through eight holes immediately downstream of the swirler vane. The fuel/air mixer is assumed to be perfectly premixed at the dump plane and the equivalence ratio is calculated to be $\phi=0.7$. The geometric swirl number, defined as the ratio of the axial flux of the tangential momentum to the product of axial momentum flux and a characteristic radius, is $S_g=0.82$. Experiments at atmospheric pressure and temperature are conducted for two different set of Reynolds number, i.e. 10144, and 13339 (based on inlet bulk velocity and hydraulic diameter).

8.1.1 Stereoscopic PIV and Measurement

For three-dimensional velocity measurements, a commercial PIV system (IDT Inc) using two Sharp Vision 1300DE cameras is used, as shown in Figure 8.1. These CCD cameras have a resolution of 1280(H) x 1024(V) pixels with pixel size of 6.7 x 6.7\(\mu\)m. Both cameras are equipped
Figure 8.2: Sectional view of the swirl injector

Figure 8.3: Close-up view of the computation grid
with Nikon lens of 50mm focal length. To illuminate the flow field of interest, laser-light from a
twin head dual cavity Nd:YAG laser is combined and frequency doubled in order to generate two
green light pulses at 532 nm., with pulse energy of 120 mJ and pulse duration of 5 ns. The laser
beam, with diameter of 5 mm, goes through the optics of a cylindrical and a spherical lens and
forms a light sheet in the measurement field. During the measurement, the PIV system is operated
at frame rate of 10 Hz. The time between two laser pulses is between 20 and 40 \( \mu s \), depending on
the flow velocity; this time increment is used to optimize the accuracy of data processing. The
field of view (FOV) is approximately 85mm x 60mm. Since this FOV is large, the lens aperture
is adjusted to ensure the appropriate image size of seeding particles for the accuracy of post data
processing. The seeding particles are small enough to ensure good tracking of the fluid motion
and big enough to scatter light for image capturing. Here TiO\(_2\) particles with nominal diameter
of 3\( \mu m \) are introduced upstream of the swirler in order to distribute them homogenously and
to follow the flow oscillation with a frequency up to 1 kHz (Melling, 1997). Although the PIV
measurements made do not resolve the 1 KHz time scale, it is important for the seeding particles
to correctly represent the instantaneous fluctuations of the flow-field.

IDT pro-VISION software offers two different algorithms to extract displacements from an
image pair: standard and adaptive interrogation modes. Here the second mode is utilized since
it is based on a second-order accurate mesh free algorithm of Lourenco and Krothapalli (2000),
which is designed to reduce or avoid such errors as loss of pairing, image truncation, and spatial
averaging of velocity gradients. Smaller interrogation windows can improve spatial resolution
of the velocity field, but also increase the probability of velocity underestimation (Lourenco
and Krothapalli, 2000). A 60x50 mesh has been then used to get 3000 vectors per frame with
32x32 correlation windows. It yields a spatial resolution of approximately 1.1x1.0 mm. Because
of the complex nature of the swirling flow field, care is taken to optimize inter-frame timing,
camera aperture setting, laser-sheet thickness, and seeding density. Using a portion of the light sheet with approximately 2.0 mm thickness and a short inter-frame time helped to freeze the out-of-plane motion of seed particles. Sets of 500 image pairs are usually recorded for each data set and statistically processed for the mean and RMS values. Considering a typical value in the measurement error of 0.1 pixel units (Westerweel, 1993), which combines bias and RMS errors, and a typical displacement of 8 pixel units in this experimental PIV measurement, this error is 1.25% as a percentage for mean local velocity.

8.2 Numerical Techniques

In this investigation, the computational method uses LES combined with a TF approach for combustion. To model the turbulent flow, LES is used where the energetic larger-scale motions are resolved, and the small scale fluctuations are modeled. Therefore, the equations solved are the filtered governing equations for the conservation of mass, momentum, energy and species transport in a curvilinear coordinate system. The sub-grid stress modeling uses a dynamic Smagorinsky model. Modeling the flame-turbulence interaction in premixed flames requires tracking of the thin flame front on the computational grid. Hence, we use the thickened flame approach which is a cost-effective strategy while allowing the chemistry to be represented. In this technique, the flame front is artificially thickened to resolve it on the computational grid while allowing the flame to propagate at the same speed as the un-thickened flame. The artificial thickening of the flame front is obtained by multiplying the diffusion term by a factor F and dividing the reaction rates by the same factor to maintain the flame speed. More detailed description of this technique is found in the literature (Chapter 4). The major advantage associated with this TF model is the ability to capture the complex swirl stabilized flame behavior which is often found in a gas turbine combustor. Since this type of geometry with the premixing section does not guarantee a perfectly premixed gas at the dump plane, the fully premixed assumption in the numerical model is not valid any more. The present TF model is capable of taking care of this
type of partially premixed gas since we solve for the individual species transport equations and
the reaction rates are specified using Arrhenius expressions.

Figure 8.4: Streamline patterns for non-reacting flow condition [D: center-body diameter]: (a) Re=10144, (b) Re=13339

8.2.1 Chemistry Model

As all the species are explicitly resolved on the computational grid, the Thickened Flame model is best suited to resolve major species. Intermediate radicals with very short time scales can not be resolved. To this end, only simple global chemistry has been used with the thickened flame model. In the present study, 2-step reaction chemistry is used.

A two step chemistry, which includes six species (CH$_4$,O$_2$,H$_2$O,CO$_2$,CO and N$_2$) is given by the following equation set.

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$$ (8.1)

$$CO + 0.5O_2 \leftrightarrow CO_2$$ (8.2)
Figure 8.5: Snapshots of vorticity magnitude field for non-reacting flow condition: (a) Re=10144, (b) Re=13339

The corresponding reaction rate expressions are given by:

\[ q_1 = A_1 \exp\left(-\frac{E^1_a}{RT}\right)[CH_4]^{a_1}[O_2]^{b_1} \]  \hspace{1cm} (8.3)

\[ q_2(f) = A_2 \exp\left(-\frac{E^2_a}{RT}\right)[CO][O_2]^{b_2} \]  \hspace{1cm} (8.4)

\[ q_2(b) = A_2 \exp\left(-\frac{E^2_a}{RT}\right)[CO_2] \]  \hspace{1cm} (8.5)

where the activation energy \( E^1_a = 34500 \text{ cal/mol}, E^2_a = 12000 \text{ cal/mol}, a_1 = 0.9, b_1 = 1.1, b_2 = 0.5, \) and \( A_1 \) and \( A_2 \) are \( 2.\times10^5 \) and \( 1.\times10^9 \), respectively, as given by Selle et al. (2004). The first reaction (Eq. 8.1) is irreversible, while the second reaction (Eq. 8.2) is reversible and leads to an equilibrium between \( CO \) and \( CO_2 \) in the burnt gases. Hence the expression (Eq. 8.3) represents the reaction rates for the irreversible reaction (Eq. 8.1) and the expressions (Eq. 8.4 & 8.5)
represent the forward and backward reaction rates for the reversible reaction (Eq. 8.2). Properties including density of mixtures are calculated using CHEMKIN-II (Kee et al., 1989) and TRANFIT (Kee et al., 1986) depending on the local temperature and the composition of the mixtures at 1 atm. In the literature by Selle et al. (2004), they have compared this two-step scheme with GRI mechanism and showed that this two-step mechanism yields fairly good comparison with respect to measured temperatures, burnt gas temperatures, major species mass fractions and flame speeds for a range of fuel-air ratios.

8.2.2 Computational Domain and Boundary Conditions

As noted earlier, and shown in Fig. 8.2, the configuration of interest in the present work is an unconfined swirling burner. The computational domain (Fig. 8.3) extends 20D downstream of the dump plane (fuel-air nozzle exit), 13D upstream of the dump plane (location of the swirl vane in Fig. 8.2) and 6D in the radial direction. Here, D is the center-body diameter. Two different LES grids are studied (for cold flow only): one that consists of 210x138x32 grid points downstream of the dump plane plus (64x23x32)+(75x17x32) grid points upstream (where the grid is in two blocks), and corresponds to approximately 1.22M grid points (mesh1: coarse). The finer mesh consists of 320x208x48 grid points downstream of the dump plane plus (98x32x48)+(114x22x48) grid points upstream, and contains approximately 3.94M grid points (mesh2: fine).

The inflow boundary condition is assigned upstream of the dump plane and corresponds to the experimental location immediately downstream of the swirler blades. The mean axial velocity distribution is specified as a one-seventh power law profile to represent the fully developed turbulent pipe flow, with superimposed fluctuations at 10% intensity levels (generated using Gaussian distribution). A constant tangential velocity component is specified as determined from the swirl vane angle. Convective boundary conditions (Akselvoll and Moin, 1996) are prescribed at the outflow boundary, and stress-free conditions are applied on the lateral boundary in order to allow the entrainment of fluid into domain. The time step used for the computation is dt=1.0e-3.
Figure 8.6: Non-reacting flow results for Re=10144 at different axial locations [r1=(r/2D) x 25.4; X2, X3, X4=(X/2D) x 25.4]: Experimental data (Δ), Lines are LES predictions: fine mesh (—), coarse mesh (– - -). Mean axial velocity U/U₀, Mean tangential velocity W/U₀, Axial velocity fluctuation u’/U₀, Tangential velocity fluctuation w’/U₀.

Figure 8.7: Non-reacting flow results for Re=13339; Legend See Fig. 8.6
8.3 Results and Discussion

We will first present the non-reacting LES calculations to ensure that the grid and boundary conditions are properly chosen, and to assess the cold-flow flow characteristics. This will be followed by a discussion of the reacting flow calculations where we will examine both the flow and heat release distributions. The measurements and simulations will be generally presented together so that a comparative assessment can be made.

![Figure 8.8: Snapshots of vorticity magnitude field for reacting flow condition: (a) Re=10144, (b) Re=13339](image)

8.3.1 Non-reacting Flow Results

Figure 8.4 shows the stream line patterns for different Reynolds number. Three distinct recirculation regions are observed in the high Reynolds number case, Re=13339, that include a separation wake recirculation zone (WRZ) behind the center body, a corner recirculation zone (CRZ) due to sudden expansion of combustor configuration, and a central toroidal recirculation zone (CTRZ) formed due to vortex breakdown. The CTRZ, however, is not prominent in the low Reynolds number case (Re=10144) and appears as an asymmetric structure that becomes more
Figure 8.9: Mean temperature field streamline patterns for reacting flow condition: (a) Re=10144, (b) Re=13339
clearly visible and symmetric at higher Reynolds number (Re=13339). The asymmetry at the lower Reynolds number indicates a low-frequency unsteadiness (Fig. 8.12) that is not averaged out despite the long integration times (15-25 flow through times) used for statistical averaging. Thus the origins of the CTRZ at the lower Re appear to be in the form of a flapping vortical structure that becomes more steady and well defined at higher Reynolds numbers. Based on these observations, at the lower Re, the WRZ and CRZ are likely to play an important role in the flame holding, while with increasing Re, the CTRZ becomes the dominant structure and will be of primary significance in the flame holding behavior. Figure 8.5 shows the snapshots of the vorticity magnitude field, and supports the observations in Fig. 8.4. It is evident that at the lower Reynolds number the large vortical structures are mostly arising from the annular shear layers, and that the center-recirculation regions do not have large vorticity. As the Reynolds number is increased, the vortex shedding in the shear layers continue to be well organized, have larger spreading angles, and vorticity levels in the wake and the center-recirculation regions increase reflecting the greater role of the central-toroidal recirculation zone.

The radial distribution of the axial and tangential mean velocity profiles, and the axial and tangential fluctuations at different axial locations are shown in Figs. 8.6 - 8.7. The time-averaged mean quantities are normalized by the corresponding bulk velocity (U_o=7.28 m/s, U_o=9.57, corresponding to Reynolds number Re=10144, and Re=13339, respectively). Results from both the coarse and fine grid are shown in the plots. In general, the agreement between LES and the experimental data is quite good with the peak velocities and turbulence levels correctly predicted both in magnitude and location. The shape, size, and the intensity of the recirculation zone (region of negative axial velocities at the center) are well predicted along with the overall spreading of the turbulent swirling jet. Some level of asymmetry can be observed in both the simulations and the experiments and indicate that the statistical averaging period needs to be carried out
over a longer period of time. However, due to the presence of low-frequency unsteadiness in the flow, the averaging time-periods can be very large and impractical from both computational and experimental perspectives. Similar observations of asymmetry in the averaged profiles have also been reported in the literature for confined combustor geometry (selle et al., 2004).

The RMS fluctuations of the axial and tangential velocities are also shown in Figs. 8.6 - 8.7. The LES predictions only report the resolved stresses, but these predictions are in good agreement with the experimental data. For example, at the highest Reynolds number (Fig. 8.77) the predicted axial fluctuations are in excellent agreement with the measured values and therefore indicate that the primary contributor to these stresses are from the larger resolved scales. The peak in the axial velocity fluctuations is observed to be in the shear layer and between the location of the peak velocity and the recirculation bubble. In this region, the steepest velocity gradient $\partial U_i/\partial x_j$ is obtained and promotes the production of the peak kinetic energy. The tangential velocity fluctuations show a flatter profile than the axial velocity fluctuations and their peaks are shifted radially inwards as for the mean tangential velocities.

For both the mean velocity and fluctuations, the fine mesh (3.94M grid points) results are in better agreement with the experimental data compared to those from the coarse mesh (1.22M grid points) for all the cases considered here. Hence, the fine mesh is chosen for reacting flow calculations later on.

8.3.2 Reacting Flow Results

Figure 8.8 shows the snapshots of the vorticity magnitude field under reacting flow conditions at different Reynolds number. Comparing to non-reacting cases (Fig. 8.5), the vortical structures have higher magnitude due to the added heat release, and the shear layers appear to be more distinct and axially-directed compared to the non-reacting case. The same features are also observed in Fig. 8.9, which shows the distinct stream line patterns corresponding to the shear layers. Compared to the corresponding streamlines for the cold flow case shown in Fig. 8.4,
Figure 8.10: Snapshots of iso-vorticity surface at $\omega=13 \text{ s}^{-1}$ for non-reacting flow (left) and reacting flow (right) conditions: (a) Re=10144, (b) Re=13339
Figure 8.11: Snapshots of Gas expansion (top), baroclinic production (middle) and diffusion term (bottom) for non-reacting (left) and reacting flow (right) conditions for Re=13339
it can be seen that the heat release distributions dramatically alter the flow patterns. Notably, the length of inner recirculation zone (both the WRZ and CTRZ) is reduced while the length of corner-recirculation zone increased quite significantly in the reacting flow field.

Contours of the mean temperature levels are superimposed on the streamlines in Fig. 8.9 and show that the highest temperatures occur along the inner edge of the shear layers and in the CTRZ. Note the inner edges of the shear layer are associated with the highest turbulence which are likely to promote molecular-level mixing and combustion.

Figure 8.10 shows the snapshots of the iso-vorticity surface at $\omega = 13 \text{ s}^{-1}$ for both reacting and non-reacting cases. It is clearly observed that for low Reynolds number case, a typical vortex spiral starts evolving from the shear layers due to Kelvin-Helmholtz instabilities in both the axial and azimuthal directions. This structure, called the PVC, precesses around the centerline and sustains for several turns before breaking down into smaller structures. For the higher Reynolds number, the spiral vortex structures are also observed; however, the structures appear to be more complex due to the higher centrifugal force and they spread more rapidly in the radial direction breaking down to form smaller scale structures.

While the PVC is clearly observed for both the non-reacting cases and reacting cases, the PVC appears more axially-elongated for the reacting cases, but suppressed radially (Fig. 8.10). To understand this behavior, it is educational to look at the terms of the vorticity transport equation which is written as:

$$\frac{D \vec{\omega}}{Dt} = \left( \nabla \times \frac{\vec{u}}{i} \right) - \frac{\vec{\omega}}{ii} \left( \nabla \times \frac{\vec{u}}{i} \right) \frac{\vec{\nabla} \rho}{\rho^2} + \nu \nabla^2 \frac{\vec{\omega}}{IV}$$ (8.6)

where the RHS terms are: (I) Vortex stretching, (II) Gas expansion, (III) Baroclinic production, and (IV) Viscous diffusion. Figure 8.11 shows these terms at one Reynolds number (13,339) for both the non-reacting and reacting flow fields. The vortex stretching term is comparable for both the reacting cases and the non-reacting cases and is not shown since it is not responsible for
the differences see in Fig. 8.10. The gas expansion term acts as a sink in reacting cases due to negative sign in the transport equation. This term is directly proportional to the gas dilatation ratio across the flame \((\rho_u/\rho_b)\), which increases as the temperature increases in presence of combustion. This term and its greater value for the reacting case (Fig. 8.11) is clearly partly responsible for the reaction-induced-damping of the PVC seen in Fig. 8.10. As the kinematic gas viscosity increases due to temperature in the flame, this substantially enhances the rate of vorticity diffusion and further damps the core vorticity. However, the pressure gradient generated due to inclination and expansion of the flame with respect to the flow field, vorticity is produced due to the baroclinic production term. The gas expansion ratio \((\rho_u/\rho_b)\) affects both the source and sink terms. In the present case, it actually gives rise to the production and gas expansion terms and diffusion term as well (Fig. 8.11). Hence, the combined effects of gas expansion, production and diffusion terms make the PVC axially elongated. Moreover, the size of the corner recirculation zone (CRZ) in Fig. 8.9 also supports the existence of the axially elongated PVC, although the effects of this exothermicity produce thicker vortical structures in the reacting cases (Fig. 8.10).

Figure 8.12 shows the frequency spectra of the velocity field at a specific location in the PVC. In both cases, the PVC oscillating frequencies are below 12 Hz. For the non-reacting case, the low frequency oscillation peaks are more clearly observed with two dominant peaks around 1.5 and 3 Hz. This clearly indicates that the PVC oscillation frequencies are suppressed with reaction.

Figure 8.13 shows the distributions of the normalized axial velocity profiles, and axial fluctuations at different axial locations. The overall agreement of the predictions with the data is found to be quite reasonable, considering the complexity of the physical processes and the configuration. Compared to the non-reacting cases, the magnitude of the velocity peak is increased and the radial-spreading angle is wider. With increasing axial distance the magnitude of the peak velocity decreases and the location of the peak is moved further outwards radially. As noted
earlier by comparing the streamline plots in Figs. 8.4 and 8.9, the negative velocities for the non-reacting cases are larger in magnitude than the reacting flow cases.

While the general agreement between the data and predictions are satisfactory, and the LES results show the right qualitative features and the peak magnitudes, there are intrinsic differences between the predictions and data. The axial velocities show a narrower shear-layer region and a small over-prediction of the peak axial velocity particularly at the upstream locations. Predicted RMS fluctuations clearly exhibit two peaks. The location of the peaks correspond to the burnt and un-burnt regions in the inner part of the shear layer and associated with the high velocity gradients where the turbulence production due to the mean velocity gradient is the highest. The first peak is lower in magnitude and located in the burnt region of the shear layer downstream of the center body where the temperatures are higher. The high temperatures cause the viscosity value to go up, and this reduces the magnitude of the peak stress component. The second peak is observed in the un-burnt regions of the shear layer where the temperatures are relatively on the lower side which reduces the viscosity value and in turn exhibits higher fluctuating components. Similar trends for RMS fluctuations have also reported by other researchers reporting calculations (Galpin et al., 2008). However, the measurements do not clearly show this dual-peak behavior.

The radial distributions of the major species mass fractions are presented in the Fig. 8.14 for Re=13339. The entrainment of ambient air is clearly observed in the distributions of O₂. Along the centerline, CH₄ and O₂ consumptions are higher which, in turn, reflect in the higher temperature zones observed earlier (Fig. 8.9). Un-burnt CH₄ is observed behind the center-body. No reacting species excluding O₂ is observed away from the flame region (r1>20 mm). Away from the dump plane (X4=40 mm) the temperature goes down; consequently the O₂ consumption level goes down. This lower temperature zone is clearly visible from Fig. 8.9 and Fig. 8.15 where the predicted mean heat release patterns show shorter flame length and lower temperature regions.
Figure 8.12: Spectrum of axial velocity fluctuations for non reacting and reacting cases for \( Re=10144 \)

Figure 8.13: Reacting flow results for \( Re=10144 \) (left), and \( Re=13339 \) (right) at different axial locations \([r1=(r/2D) \times 25.4; \, X2, \, X3, \, X4=(X/2D) \times 25.4]\): Experimental data (\( \Delta \)), Lines are LES predictions (—). Axial velocity \( U/U_0\), Axial velocity fluctuation \( u'/U_0\).
Figure 8.14: Mean species concentration for $Re=13339$ at different axial locations [$r_1=(r/2D) \times 25.4$; $X_1$, $X_2$, $X_3$, $X_4=(X/2D) \times 25.4$]: $\text{CH}_4$ (---), $\text{O}_2$ (- - -), $\text{H}_2\text{O}$ (---), $\text{CO}_2$ (· -- ·), 10x$\text{CO}$(——)
Figure 8.15: Experimental CH chemiluminescence measurement (left), Computational mean heat release (W/m$^3$) predictions at center plane (middle), Computational mean heat release (W/m$^3$) predictions averaged across flame (right): (a) Re=10144, (b) Re=13339

Figure 8.16: Turbulent kinetic energy predictions: (a) Re=10144, (b) Re=13339
8.3.2.1 CH-chemiluminescence Measurement

CH radicals are produced at the flame front and represent the reaction zones. Therefore CH chemiluminescence imaging has been carried out in the present work. An intensified Princeton Instruments PI-MAX 512 T-18 G/III CCD camera with a 512x512 pixel solution has been utilized to acquire such images. A filter mounted on the camera lens is used to transmit the light at $\lambda=430$ nm which corresponds to the $B2\Sigma^+-X2\Pi(0,0)$ emission band of the CH radical (Garland and Crosley, 1985) and to attenuate all other wavelength contributions. Gain is adjusted based on the operating condition and the gate duration for the image acquisition is set to 400$\mu$s. The CH images are processed with corresponding background images and averaged over their whole sequence of 336 images. The averaged results are shown in the Figure 8.15 (left). CH chemiluminescence is here considered to representative of the heat release rate. Also shown in Fig. 8.15, are the predicted heat release distributions along the center plane (middle) and averaged across the flame (right). It should be noted that the CH data and the predicted heat release distributions while related to each other are not directly the same quantity and can only be qualitatively compared with each other, and show reasonable agreement (compare the averaged measured image on left with the averaged predicted image on the right in Fig. 8.15).

Figure 8.15 shows that the CH distributions and the heat release patterns are similar to each other, in that, the levels are highest in the inner-regions of the shear layer. It can be seen that as Reynolds number increases the turbulent flame becomes more compact and exhibits its peak CH signal closer to the dump plane. This is seen in both the experimental and computational distributions. It is observed experimentally that the flame is slightly lifted off at the highest Reynolds number; however, computations show a more compact flame and shorter flame length (also seen in mean velocity predictions, Fig 8.13). A higher Re tends to increase the turbulence intensity and the flame speed as well, and consequently shortens the flame length.

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Figure 8.16 shows the predicted turbulent kinetic energy (TKE) contours. Further, as Re increases, high turbulence enhances the interaction between flame-turbulence; resulting in higher heat release, which, in turn, affects the turbulent kinetic energy patterns. Turbulent kinetic energy (TKE) contours also show that the TKE is lower in the higher temperature regions and increases in the lower temperature regions. The lower and higher TKE plots explain the double peak captured in the RMS fluctuations of the axial velocity (Figs. 8.13).

8.4 Conclusions

PIV measurements and LES with a TF model are used to investigate unconfined swirling flows in a laboratory based model combustor. Both reacting and non-reacting flow conditions for different Reynolds numbers are studied. A 2-step chemical scheme is invoked to represent the flame chemistry for methane-air combustion. The equivalence ratio for the flame is 0.7 and the geometric swirl number for the configuration is 0.82. CH chemiluminescence imaging is also carried out to characterize the heat release distributions.

Isothermal flow predictions are in good agreement with the measurements and indicate that the boundary conditions and grid are properly chosen. Reynolds number is seen to have an impact on the flow field particularly for the non-reacting cases. At a high Re, all the recirculation zones, such as WRZ, CRZ and CTRZ (caused due to vortex breakdown), are clearly observed. At lower Re, the CTRZ is a weaker structure that exhibits a low-frequency unsteady flapping.

For the reacting flows, the mean axial velocity profiles are in good agreement with measurements, and slightly over-predicted close to the dump plane locations. This over-prediction is reflected by a more compact and attached flame in the predictions compared to the experimental observations which show a slightly lifted flame. Moreover, the predicted RMS fluctuations exhibit double peak in the burnt and un-burnt regions and on either side of the peak heat release.

The measured and predicted heat release distributions are in qualitative agreement with each other and exhibit the highest values along the inner edge of the shear layer. With increasing
Reynolds number the flame region is seen to be more compact both experimentally and computationally.

This study demonstrates that the Thickened-Flame based LES approach with simplified chemistry for reacting flows is a promising tool to investigate reacting flows in complex geometries.
Chapter 9  Flashback in Hydrogen Enriched Premixed Combustion

In recent times, ‘Clean Coal Combustion’ has gained considerable attention as the favored method for clean power generation in stationary gas turbines. Hence, syngas is used as an obvious fuel of choice, which is obtained from coal gasification and contains hydrogen (H₂) as a primary component. However, this composition largely depends on the gasification process and plays a significant role in characterization of the flame behavior. Therefore it is desirable to understand how mixing of natural gas and syngas in different proportions effects the combustion characteristics. As a consequence this leads to design issues of syngas combustor in order to handle the variabilities in fuel composition without requiring any design changes (Calvetti et al., 2001). This is the primary reason why fuel flexibility poses much of a design challenge. Nevertheless, the issues of interest in premixed combustion are to operate the combustor in a safe, efficient, and reliable manner. This means the flame neither flashes back nor blows out, and the fuel is burned in a steady fashion. However, the major operability issues associated with lean premixed combustions are: flame-holding, flashback, combustion instabilities and auto-ignition.

In order to achieve stable combustion, hydrogen doping appears to be a promising approach to increase the Lean-Blow-Out (LBO) limits of hydrocarbon fuels (Griebel et al., 2007). In this operating range, flame holding becomes an important issue of consideration for the combustor, although this can be avoided by increasing the hydrogen proportion in the fuel. Increase in hydrogen proportion will assure better flame stability but, at the very same time, it will make the combustor more susceptible to flashback and thermo-acoustic instability.

On the other hand, flashback becomes an inherent problem in this type of system due to addition of hydrogen, since hydrogen flame speeds are quite high (Mariotti et al., 2002). It is an intrinsic behavior of premixed systems as the flame stabilizes at upstream of the combustion
chamber. Flashback has been extensively investigated by several researchers (Wohl, 1952; Plee et al, 1978; Putnam et al, 1948) and they reported that the complexity of the topic becomes more substantial in swirling flows (Noble et al., 2006). There are several explanations found in the literature (Fritz et al., 2004; Kröner et al., 2003; Kiesewtter et al., 2004), but the occurrence of flashback is unique to each system. Flashback may occur due to different reasons as discussed below:

- **Flashback by Flame Propagation**

Flashback occurs when the flow velocity is of the same order as the burning velocity, so that the flame is able to propagate upstream of the combustion chamber. The sufficiently low velocity in the boundary layers also allows flame to propagate upstream of the combustion chamber and causes flashback. However, wall quenching can limit this behavior to some extent for non-industrial and laminar configurations. The wall velocity gradient, laminar flame speed and quenching distance can be related for laminar flows as:

\[
g = -\frac{\partial u}{\partial r} \bigg|_R = \frac{S_L}{d_q}
\]

(9.1)

where \( g \) is the velocity gradient at the wall, \( S_L \) is the laminar flame speed, and \( d_q \) is the quenching distance. According to this criterion, \( g < S_L/d_q \) leads to upstream flame propagation near the wall. Plee et al. (1978) proposed a dimensionless relation between the downstream convective transport and the upstream flame propagation with heat loss to the wall. However, the known fact is that the same criteria can not be applied to turbulent boundary layers. Flashback in boundary layers seems to be predominant in non-swirling low turbulent flows or low-speed catalytic combustion (Sommerer et al., 2004).

Flashback occurs when the turbulent flame speed becomes higher than the local flow velocity and the flame propagates upstream of the system. The turbulent burning velocity mainly depends
on the chemical kinetics and the turbulent structure, i.e. the length scales and the local velocity fluctuations. However, the determination of turbulent burning velocity remains a challenging task due to complex interaction of turbulence and chemistry. This situation is more prominent in swirling flames, where intensity of the turbulence is higher and the available flame surface is significantly larger than the laminar flame surface leading to the occurrence of flashback. Furthermore, at moderate mixture temperature for stable fuels like natural gas, flashback in the core flow is less critical even in highly turbulent flows due to the low laminar flame speed.

- **Flashback Due to Combustion Instabilities**

  Combustion instabilities are caused due to the coupling between volumetric heat release, pressure fluctuations and flow hydrodynamics. As the induced velocity fluctuations due to instabilities become as large as the mean velocity lead to transient flashback during the oscillation cycle. These instabilities can also be responsible for the upstream flame propagation, both in boundary layers and in the core flow as well. Swirled burners being more sensitive to such instabilities, may become prone to triggering the flashback in these type of combustors. However, the fluctuations required to cause such problems are beyond the acceptable noise levels in most combustion systems.

- **Flashback by Vortex Breakdown**

  Vortex breakdown in swirled burner occurs when the azimuthal velocity becomes larger than the axial velocity. Moreover, this vortex breakdown is often accompanied by a large recirculation zone with high reverse flow velocities in combustions systems, and the reverse velocities can promote upstream flame propagation and flashback is the consequence. The formation of vortex breakdown strongly depends on the geometry, and if the swirl number exceeds a critical value the recirculation zone is able to extend itself throughout the entire mixing section. In isothermal flows, this effect can be prevented by selecting the swirl number; however, the chemical reaction
can nevertheless lead to a breakdown of the flow, combined with upstream flame propagation. This mechanism is called as combustion-induced vortex breakdown (CIVB) as reported by Fritz et al. (2004), Sommerer et al. (2004). Normally, swirled burner and center-body less swirl stabilized flame are more susceptible to this kind of problem. Recent studies by Nauert et al. (2007), Kiesewetter et al. (2003, 2007), Kröner et al. (2003, 2007), Knole et al. (2008), Konle and Sattelmayer (2009), Voigt et al. (2009) also reported this CIVB driven flashback in swirled burner. Flashback into the pre-mixer section leads to thermal overload and destruction of the hardware therefore it must be avoided at all load conditions (Kiesewetter et al., 2003). Flashback can be prevented by using specially designed flame holders or by injecting syngas in a separate non-premixed arrangement. However, in transitioning from natural gas as the fuel of choice to syngas, it is desirable to keep hardware changes to a minimum, given the extensive body of knowledge with current natural gas related hardware.

In addition, another important factor in stable combustion systems is fuel-air mixing. Changes in fuel-air mixing can lead to the reduction of pollutants, improved combustor efficiency, reduced combustor size, longer engine lifetimes and greater stability or operability. Many mixing enhancement techniques have been investigated and successfully used over the years. It is well known by now that premixed combustor designs often involve a trade-off between geometry and combustion performance, but the basic geometry generally involves cross-flow mixing (mixing generated by a fuel jet injected with a cross-flow) that utilizes swirl vanes at the inlet section to promote the mixing and provide improved flame holding. Moreover, cross flow mixing is found to be convenient and efficient due to its effectiveness and simplicity. The degree and rate of the mixing process is especially important in combustion applications since exhaust composition directly depends on mass transfer and reaction kinetics.

In turbulent premixed combustion, a popular approach is to rely on the flamelet concept, which
essentially assumes the reaction layer thickness to be smaller than the smallest turbulence scales. The two most popular model based on this concept are the flame surface density model (FSD) (Hawkes and Cant, 2001) and the G-equation model (Williams, 1985; Peters, 2000; Düsing et al., 2006). It has been reported that the FSD model is not adequate beyond the corrugated flamelet regime (Düsing et al., 2006, Pitsch et al., 2002), while the G-equation approach depends on a calculated signed-distance function that represents an inherent drawback of this method.

Another family of models relies on the probability density function (PDF) approach (Pope, 1985). This is a stochastic method, which directly considers the probability distribution of the relevant stochastic quantities in a turbulent reacting flow. The PDF description of turbulent reacting flow has certain theoretical benefits; the complex chemistry is taken care of without applying any ad-hoc assumptions (like ‘flamelet’ or ‘fast reaction’). Moreover, it can be applied to non-premixed, premixed, and partially premixed flames without having much difficulty. However, the major drawback of the PDF transport approach is its high dimensionality, which essentially makes the implementation of this approach to different numerical techniques, like FVM (Finite Volume Method) or FEM (Finite Element Method), limited.

In this work, a Thickened Flame (TF) model (Colin et al., 2000) is invoked where the flame is artificially thickened to resolve it on computational grid points where reaction rates from kinetic models are specified using reduced mechanisms. The influence of turbulence is represented by a parameterized efficiency function. A key advantage of the TF model is that it directly solves the species transport equations and uses the Arrhenius formulation for the evaluation of the reaction rates.

The major advantage associated with this TF model is the ability to capture the complex swirl stabilized flame behavior which is often found in a gas turbine combustor. Since this type of geometry with the premixing section does not guarantee a perfectly premixed gas at the dump
plane, the fully premixed assumption in the numerical model is not valid any more. The present TF model is capable of taking care of this type of partially premixed gas since we solve for the individual species transport equations and the reaction rates are specified using Arrhenius expressions.

The configuration of interest in the present work is hydrogen-enriched swirl-stabilized flame. Several studies have investigated premixed flames of H₂-hydrocarbon fuel mixtures. Recent examples include studies by Morris et al. (1998) of commercial gas turbine engine operating in the LPM combustion mode, Schefer (2003), Schefer et al. (2002), Kim et al. (2009), Ballester et al. (2009) of swirling hydrogen-enriched flames, Griebel et al. (2007) of hydrogen-enriched flames at higher pressure, Strakey et al. (2007) of swirl stabilized hydrogen-enriched flames at high pressure. Moreover, Kröner et al. (2003, 2007) also reported flashback due to combustion induced vortex breakdown (CIVB) in swirling flows for different CH₄+H₂ mixtures. They reported that the CIVB happened to be the prevailing mechanism in a swirled burner without center-body. Tuncer et al. (2009) also investigated flashback characteristics in a confined premixed hydrogen-enriched methane flames for a laboratory scale swirled combustor. Furthermore, an extensive review on swirling flows can be found in the literature (Schneider et al., 2005; Syred and Beer, 1974; De et al., 2009). It is well known that the mixing and flame stability can be improved by varying the swirl strength. At the same time the swirl stabilized combustors encounters problems due to vortex breakdown, which forms recirculation zone and thus brings the hot products back to reactants results in triggering of flame flashback in presence of hydrogen. However, despite several years of research, the mechanisms of vortex breakdown are only partially understood (Syred and Beer, 1974; Syred, 2006; Duwig et al., 2007).

In this investigation, we study flashback in hydrogen enriched premixed swirling flames using LES combined with a TF approach for combustion. Specific goal of this study is to understand the
flashback behavior in swirling flames, and in particular, how hydrogen enrichment influences this flashback behavior.

![Diagram of a swirling premixed combustor]

Figure 9.1: A schematic of swirling premixed combustor.

### 9.1 Flow Configuration

The configuration considered here is an unconfined swirl burner as shown in Fig. 9.1. The 45° swirl vane (9.2) is fitted with a solid center body which also acts as a fuel injector (Fig. 9.1). This center body extends beyond the swirl vane and is flush with the dump plane of the combustor. The diameter of the center body is 12.7mm (0.5 inch) and the O.D. of the swirler is 34.9 mm (1.375 inch). Methane and hydrogen gas is injected radially from the center body through eight holes immediately downstream of the swirler vane. The fuel/air mixer is assumed to be perfectly premixed at the dump plane and the equivalence ratio is calculated to be $\phi=0.7$. The geometric swirl number, defined as the ratio of the axial flux of the tangential momentum to the product of axial momentum flux and a characteristic radius, is $S_g=0.82$. The investigation is carried out for Reynolds number, $Re=10144$ (based on inlet bulk velocity and hydraulic diameter) at atmospheric pressure and temperature.
9.1.1 Numerical Details

In this investigation, the computational method uses LES combined with a TF approach for combustion. To model the turbulent flow, LES is used where the energetic larger-scale motions are resolved, and the small scale fluctuations are modeled. Therefore, the equations solved are the filtered governing equations for the conservation of mass, momentum, energy and species transport in a curvilinear coordinate system. The sub-grid stress modeling uses a dynamic Smagorinsky model. Modeling the flame-turbulence interaction in premixed flames requires tracking of the thin flame front on the computational grid. Hence, we use the thickened flame approach which is a cost-effective strategy while allowing the chemistry to be represented. In this technique, the flame front is artificially thickened to resolve it on the computational grid while allowing the flame to propagate at the same speed as the un-thickened flame. The artificial thickening of the flame front is obtained by multiplying the diffusion term by a factor F and dividing the reaction rates by the same factor to maintain the flame speed. More detailed description of this technique is found in the literature (Chapter 4). The major advantage associated with this TF model is the ability to capture the complex swirl stabilized flame behavior which is often found in a gas turbine combustor. Since this type of geometry with the premixing section
Figure 9.3: Close up view of the computational domain
does not guarantee a perfectly premixed gas at the dump plane, the fully premixed assumption in the numerical model is not valid any more. The present TF model is capable of taking care of this type of partially premixed gas since we solve for the individual species transport equations and the reaction rates are specified using Arrhenius expressions.

Figure 9.4: Non-reacting flow results for Re=10144 at different axial locations [D=Center-body diameter]: Experimental data (Δ), Lines are LES predictions: fine mesh (—, blue solid lines ), coarse mesh (---, purple dashed lines ). Mean axial velocity $U/U_o$, Mean tangential velocity $W/U_o$, Axial velocity fluctuation $u_{rms}/U_o$, Tangential velocity fluctuation $w_{rms}/U_o$

### 9.1.1.1 Chemistry Model

As all the species are explicitly resolved on the computational grid, the Thickened Flame model is best suited to resolve major species. Intermediate radicals with very short time scales can not be resolved. To this end, only simple global chemistry has been used with the thickened flame model.

For CH₄ combustion a two step chemistry, which includes six species (CH₄,O₂,H₂O,CO₂,CO and N₂) is given by the following equation set.
\[ CH_4 + 1.5O_2 \rightarrow CO + 2H_2O \]  \hspace{1cm} (9.2)

\[ CO + 0.5O_2 \leftrightarrow CO_2 \]  \hspace{1cm} (9.3)

To incorporate \( H_2 \) reaction in addition to the above \( CH_4 \) chemistry, the following 1-step Marinov mechanism is employed.

\[ H_2 + 0.5O_2 \rightarrow H_2O \]  \hspace{1cm} (9.4)

The corresponding reaction rate expressions are given by:

\[ q_1 = A_1 e^{x(-E_{a1}^{1}/RT)}[CH_4]^{a1}[O_2]^{b1} \]  \hspace{1cm} (9.5)

\[ q_2(f) = A_2 e^{x(-E_{a2}^{2}/RT)}[CO][O_2]^{b2} \]  \hspace{1cm} (9.6)

\[ q_2(b) = A_2 e^{x(-E_{a2}^{2}/RT)}[CO_2] \]  \hspace{1cm} (9.7)

\[ q_3 = A_3 e^{x(-E_{a3}^{3}/RT)}[H_2][O_2]^{b3} \]  \hspace{1cm} (9.8)

where the activation energy \( E_{a1}^{1} = 34500 \text{ cal/mol}, E_{a2}^{2} = 12000 \text{ cal/mol}, a1=0.9, b1=1.1, b2=0.5, \)
and \( A_1 \) and \( A_2 \) are 2.e+15 and 1.e+9, respectively, as given by Selle et al. (2004), and \( E_{a3}^{3} = 35002 \)
\text{ cal/mol}, \( b3=0.5, A_3=1.8e+16 \) (SI units) as given in the DOE report (DE-FC26-03NT41893, 2005). The first and third reactions (Eqs. 9.2 & 9.4) are irreversible, while the second reaction (Eq. 9.3) is reversible and leads to an equilibrium between CO and \( CO_2 \) in the burnt gases. Hence the expressions (Eqs. 9.5 & 9.8) represent the reaction rates for the irreversible reactions (Eqs. 9.2 & 9.4) and the expressions (Eq. 9.6 & 9.7) represent the forward and backward reaction.
rates for the reversible reaction (Eq. 9.3). Properties including density of mixtures are calculated using CHEMKIN-II (Kee et al., 1989) and TRAFIT (Kee et al., 1986) depending on the local temperature and the composition of the mixtures at 1 atm.

### 9.1.1.2 Computational Domain and Boundary Conditions

As noted earlier, and shown in Fig. 9.1, the configuration of interest in the present work is an unconfined swirled burner. The computational domain (Fig. 9.3) extends 20D downstream of the dump plane (fuel-air nozzle exit), 13D upstream of the dump plane (location of the swirl vane in Fig. 9.1) and 6D in the radial direction. Here, D is the center-body diameter. The finer mesh consists of 320x208x48 grid points downstream of the dump plane plus (98x32x48) + (114x22x48) grid points upstream, and contains approximately 3.94M grid points (De et al., 2009). The grid resolution in the computational domain with 3.94M grid points is given as: (a) along axial direction \( \Delta x/2D=0.031 \) is maintained from inlet to dump plane, and then 0.03125 rest of the whole domain starting from dump-plane to outlet, (b) along the radial direction \( \Delta r/2D=0.014-0.0145 \) is maintained starting from centerline to lateral boundary, (c) along azimuthal direction: behind center-body \( \Delta \theta/2D=0.011-0.0327 \) (up to \( r/2D=0.25 \)), in the annular shear layer \( \Delta \theta/2D=0.0327-0.089 \) (\( r/2D=0.25-0.6875 \)), and finally \( \Delta \theta/2D=0.089-0.393 \) (\( r/2D=0.6875-3.0 \)) where D=center-body diameter. The close-up view of the computation grid is shown in Fig. 9.3. More details on computation grid can be found in the literature (De et al., 2009).

The inflow boundary condition is assigned at the experimental location immediately downstream of the swirler blades. The mean axial velocity distribution is specified as a one-seventh power law profile to represent the fully developed turbulent pipe flow, with superimposed fluctuations at 10% intensity levels (generated using Gaussian distribution). A constant tangential velocity component is specified as determined from the swirl vane angle. Convective boundary conditions (Akselvoll and Moin, 1996) are prescribed at the outflow boundary, and symmetry
Figure 9.5: Stream line contours superimposed with axial velocity at different H₂%
Figure 9.6: Swirl number (top) and recirculation bubble size (bottom) at different H₂% [X1, X2, X3, X4=(X/2D): 0.40, 0.79, 1.18, 1.58 ]
Figure 9.7: Reacting flow results for Re=10144 with 30%H₂ at different axial locations: Experimental data (Δ), Lines are LES predictions: Mean axial velocity $U/U_0$, Axial velocity fluctuation $u_{rms}/U_0$.
Figure 9.8: Time averaged temperature contours (K scale) at different H₂%
Figure 9.9: Instantaneous flame front for CH₄ & 30%H₂ (temperature in K scale)
boundary conditions are applied on the lateral boundary. The time step used for the computation is \( dt=1.0\times 10^{-3} \). The fuel injection point is shown in Fig. 9.3, which represents a jet-in-cross flow type configuration.

9.2 Results and Discussion

We will first report the non-reacting LES calculations to ensure that the grid and boundary conditions are properly chosen, and to assess the cold-flow flow characteristics. This will be followed by a discussion of the reacting flow calculations where we will examine both the flow and flashback behavior in the context of \( \text{H}_2 \) addition.

9.2.1 Non-reacting Flow Results

Figure 9.4 shows the radial distribution of axial and tangential mean velocity profiles, axial and tangential velocity fluctuations at different axial locations for \( \text{Re}=10144 \). In general, LES and the experimental data for radial distribution of the axial and tangential mean velocity profiles, and the axial and tangential fluctuations at different axial locations are found to be in good agreement. It is observed that the shape, size, and the intensity of the recirculation zone (region of negative axial velocities at the center) are well predicted along with the overall spreading of the turbulent swirling jet. Some level of asymmetry can be observed in both the simulations and the experiments and indicate that the statistical averaging period needs to be carried out over a longer period of time. However, due to the presence of low-frequency unsteadiness in the flow, the averaging time-periods can be very large and impractical from both computational and experimental perspectives (De et al., 2009). Similar observations of asymmetry in the averaged profiles have also been reported in the literature for confined combustor geometry (Galpin et al., 2008). Also, the RMS fluctuations of the axial and tangential velocities are in good agreement with the experimental data. The peak in the axial velocity fluctuations is observed to be in the shear layer and between the location of the peak velocity and the recirculation bubble. In this region, the steepest velocity gradient \( \partial U_i/\partial x_j \) is obtained and promotes the production of the peak
kinetic energy. The tangential velocity fluctuations show a flatter profile than the axial velocity fluctuations and their peaks are shifted radially inwards as for the mean tangential velocities. More detailed discussion on non-reacting flow results can be found in the literature by De et al. (2009).

For both the mean velocity and fluctuations, the fine mesh (3.94M grid points) results are in better agreement with the experimental data compared to those from the coarse mesh (1.22M grid points) for all the cases considered here. Hence, the fine mesh is chosen for reacting flow calculations later on.

![Figure 9.10: Frequency spectra at the upstream of the dump plane](image)

### 9.2.2 Reacting Flow Results

Figure 9.5 shows stream line contours superimposed with normalized axial velocity. Evidently, it is observed that the effect of reaction and heat-release dramatically alters the flow behavior in these cases. As observed, the axial velocity contours are affected due to varying hydrogen percentage with methane fuel, and in particular, the size and strength of the recirculation bubble decreases with the increase in H$_2$% (Fig. 9.6). This can be associated with the higher
Figure 9.11: Pressure fluctuations at the upstream of the dump plane

combustibility of hydrogen which, in turn, promotes faster reaction along the flame front and results in increased temperature in that region. Also, the observed axial velocity magnitude increases by 30-35% (CH₄ to 30%H₂) and 40-45% (CH₄-50%H₂) along the flame front due to higher hydrogen addition to the methane fuel. The higher reaction rates result in increased temperature and thus the peak density (ρ) decreases ~25% (CH₄ to 30%H₂) and ~28% (CH₄-50%H₂) in this region, increasing the axial velocity by a factor of 1/ρ. On the other hand, the tangential velocity (Vₜ) increases only by ρ⁻¹/₂ to maintain the radial pressure gradient in the radial momentum equation: ρVₜ²/r = dP/dr. Because of this, the swirl ratio decreases by ρ¹/₂ as shown in (Fig. 9.6). Similar kind of observations is also reported by Kim et al. (2009) in their study.

The radial distributions of mean axial velocity and axial velocity fluctuations are shown in Fig. 9.7 for 30%H₂ mixture. The overall agreement of the predictions with the data is found to be quite reasonable, considering the complexity of the physical processes and the configuration. With
Figure 9.12: Instantaneous flame movement at phases 1-5 of oscillation frequency (45Hz) before flashback with 30%H2: stream lines colored with temperature contours (K scale)
Figure 9.13: Axial velocity fluctuations at further downstream (wrinkled flame location) of dump plane

Figure 9.14: Axial velocity spectra (12.5-17.5s) at further downstream (wrinkled flame location) of dump plane
increasing axial distance the magnitude of the peak velocity decreases and the location of the peak is moved further outwards radially. While the general agreement between the data and predictions are satisfactory, and the LES results show the right qualitative features and the peak magnitudes, there are intrinsic differences between the predictions and data. The axial velocities show a small over-prediction of the peak axial velocity particularly at the upstream locations. Predicted RMS fluctuations clearly exhibit two peaks. The location of the peaks correspond to the burnt and un-burnt regions in the inner part of the shear layer and associated with the high velocity gradients where the turbulence production due to the mean velocity gradient is the highest. The first peak is lower in magnitude and located in the burnt region of the shear layer downstream of the center body where the temperatures are higher (Fig. 9.8). The high temperatures cause the viscosity value to go up, and this reduces the magnitude of the peak stress component. The second peak is observed in the un-burnt regions of the shear layer where the temperatures are relatively on the lower side which reduces the viscosity value and in turn exhibits higher fluctuating components. Similar trends for RMS fluctuations have also reported by other researchers reporting calculations (Galpin et al., 2008). However, the measurements do not clearly show this dual-peak behavior.

Figure 9.8 shows the time-averaged temperature profiles at different hydrogen percentage
added to the fuel. It is noteworthy that the flame flashback occurs at higher H₂% and the flame moves upstream of the dump plane to premixing section and stabilizes there. This is also associated with the higher combustibility of H₂ that helps to promote faster reaction and the flame flashback is the consequence. The detailed discussion on flashback is provided in the following section.

9.2.2.1 Flashback

Figure 9.9 shows the time series temperature plots for CH₄ and 30%H₂, which clearly shows how flame propagates upstream and finally stabilizes in the mixing tube, especially for 30%H₂ mixture. For CH₄, the flame front also moves little bit upstream of the dump plane but does not move further upstream as observed in Fig. 9.9. Upstream flame propagation, usually characterized as flame flashback, occurs when the burning velocity exceeds the local flow velocity. The possible mechanisms behind flashback are discussed in the earlier section. In the present case, the flashback is initiated due to Combustion Induced Vortex Breakdown (CIVB) and then accompanied with the favorable condition, due, in part, low velocity in B/L and higher local burning velocity. As the flame starts moving upstream, especially for 30%H₂, it encounters fuel rich region due to the fuel injection point, and that induces higher flame propagation velocity in presence of highly combustible H₂. More often, the CIVB refers to the vortex break down due to chemical reaction which becomes more intensive in presence of H₂. Additionally, this vortex breakdown is often accompanied by a large recirculation zone with high reverse flow velocities in combustions systems, and the reverse velocities can promote upstream flame propagation and flashback is the consequence (Fig. 9.9).

Notably, the formation of recirculation zone is the consequence of vortex breakdown. Usually, the recirculation bubbles bring the heat and reactive species back to the flame tip and provides flame-holding at the dump plane. However, the recirculation zone gives rise to the azimuthal vorticity component in this region and that produces positive or negative induced velocity
Figure 9.16: Instantaneous flame movement during flashback with 30%H₂: Stream lines colored with temperature contours (K scale), isotherms (black lines: 300K, 675K, 1050K, 1425K)
Figure 9.17: Instantaneous flame movement with CH₄: Stream lines colored with temperature contours (K scale), isotherms (black lines: 300K, 675K, 1050K, 1425K)
following the Bio-Savart law, as give by Eq. 9.12 (Kiesewetter et al., 2007; Knole et al., 2008) depending on the sign of azimuthal vorticity. The position and motion of this recirculation bubble largely depends on the balance maintained between the induced velocity and irrotational axial velocity. Slight changes in the flow field can alter this balance and result in the upstream movement of the recirculation bubble. This unsteady motion of recirculation bubble (shown in Fig. 9.12) actually promotes the upstream flame propagation in the mixing tube, and thereafter it is accompanied by the higher induced negative velocity due to production of negative azimuthal vorticity. Fig. 9.10 shows the frequency spectra obtained from pressure fluctuations (Fig. 9.11) at the upstream of dump plane. As observed, CH$_4$ shows a peak around 62 Hz, and 30%H$_2$ shows peak around 45 Hz & 8 Hz including several others in-between 10-25Hz, while 50%H$_2$ also shows similar behavior but with higher amplitude. The observed 8Hz frequency is the bulk-mode frequency ($f = c/2\pi\sqrt{S/Vl} \sim 8.25Hz$) of the inlet delivery tube. That’s why it appears in all the cases, while the other observed frequencies are the consequence of complex interaction between recirculation bubble, flame front and jet-in-cross flow fuel injection systems. This fact will be discussed in the next paragraph in greater details.

The time series pressure fluctuations (Fig. 9.11) support the observed frequencies in Fig. 9.10. As observed in Fig. 9.10, especially for 30% & 50%H$_2$, the 45Hz frequency corresponds to the initial high amplitude oscillations where the flame propagation to the upstream is initiated due to unsteady motion of the recirculation bubble (Fig. 9.12). The initial pressure fluctuations (Fig. 9.11), especially for 30% & 50%H$_2$, correspond to the complex interaction between shedding vortices at bluff-body and motion of recirculation bubble formed due to vortex breakdown; and thereafter the fluctuations disappear at later time instants as the flame front moves upstream (flashback occurs) (Syred, 2006). Fig. 9.12 shows five different time instants representing phases during a complete cycle of the observed oscillation frequency (45Hz), and the data at each phase
Figure 9.18: Pressure ($p_o=101325$ Pa), density and baroclinic production plots during flashback with $30\%$H$_2$
Figure 9.19: Individual terms of vorticity transport equation (Eq. 9.9) during flashback with 30%H₂: stream lines (purple lines), isotherms (black lines)
is averaged over four of these cycles in order to eliminate turbulent fluctuations arising from high frequency oscillations. Stream lines colored with temperature contours are shown in Fig. 9.12 for five different phases. As observed at phase1 (Fig. 9.12), a big recirculation bubble is already formed and another small vortex (shedding vortex-1) starts forming due to shedding at the bluff-body, which also belong to inner part of another bubble whose one end has already extended into the upstream mixing tube forming a stagnation point-1 along the bluff-body wall in the upstream section whilst pressure tends to build up and causes flow reversal. At phase2 (Fig. 9.12), the same shedding vortex (shedding vortex-1) extends into the other side of the bluff-body forming another stagnation point-2 on that side while at the same time grows into a bigger vortex and starts interacting with the bubble. Moreover, formation of a saddle point is also observed at the same phase (phase-2) while the stagnation point-1 has moved further upstream due to occurrence of reverse flow as pressure reaches peak value in between phase1 and phase2. At phase3 (Fig. 9.12) the shedding vortex-1 has sufficiently grown to form almost a circulation bubble while another vortex (shedding vortex-2) starts forming form the saddle point that itself has even turned into vortex and forms a new stagnation point-3. At phase4 (Fig. 9.12) the saddle point vortex and the shedding vortex-2 merge into a single one as well as initiates to shed another new vortex from the stagnation point-3. As pressure reaches minima in between phase3 and phase4, forward flow pushes the saddle point further downstream and disappears in phase4. At phase5 (Fig. 9.12) the initiated vortex from phase4 starts growing and the cycle shows the repeatability of phase1. This unsteady interaction at the initial stage helps to push the flame front into the upstream mixing tube, especially for 30%H2 & 50 %H2, and thereafter other favorable conditions promotes the further upstream propagation. However, it should be noted that the upstream flame movement is also initiated in CH4 case (~62 Hz), but it is not supported by any favorable condition that can promote flashback resulting a limit cycle behavior in pressure fluctuations (Fig. 9.11). Fig. 9.16 shows the
flame movement in the mixing tube during flashback for 30%H₂ case. The key observation here is that the flame front is nicely stable close to the dump plane at t=8s and there is no interaction between flame front and jet-in-cross flow fuel injection. As the flame front moves further upstream at t=10.5s it starts interacting with the fuel injection system due to increase in pressure ahead of flame front (Fig. 9.18). The pressure difference between upstream and downstream of flame front (Fig. 9.18) causes the formation of a small recirculation bubble ahead of flame front, which becomes more prominent later time instants at t=12.0s & t=13.8s (Fig. 9.16). This interaction can be correlated with the lower amplitude pressure fluctuations observed between 10-13s in Fig. 9.11 where the initial high amplitude fluctuations correspond to the dynamics shown in Fig. 9.12 with a quasi-stable flame (t=8s in Fig. 9.16). Whereas similar fact is also observed in case of pure CH₄ (Fig. 9.17) and 62Hz frequency (Fig. 9.10) corresponds to the high amplitude limit cycle behavior observed in Fig. 9.11. Here, the flame front also moves little bit upstream into the mixing tube and tends to interact with the fuel injection system (Fig. 9.17) and form a small recirculation bubble ahead of flame front (like 30%H₂) at t=13.4s (Fig. 9.17). Since the further upstream movement of the flame front is annihilated due to unfavorable condition, the flame front is actually pushed back by the incoming flow (t=13.8s & t=17.6s in Fig. 9.17) and the formed small recirculation bubble (t=13.4s in Fig. 9.17) also disappears at t=13.8s & t=17.6s (Fig. 9.17). This back-n-forth movement of the flame front creates a quasi stable situation without occurrence of flashback for CH₄ and produces the limit cycle behavior in the pressure fluctuations observed in Fig. 9.11.

Figure 9.13 shows the axial velocity fluctuations at further downstream of dump plane. The velocity fluctuations in Fig. 9.13 also produce same frequency (Fig. 9.10) but disappears at later time instants as observed in the axial velocity spectra in Fig. 9.14 where Strouhal number is calculated as \( St = f D/U_o \) (D=center-body diameter, \( U_o \)= inlet bul velocity). In addition, the velocity fluctuations (Fig. 9.13) show some wavy pattern with a time period of ~1s (30%H₂). The
corresponding frequency appears to be the order of 1 Hz. This is coming due to the interaction of flame front with counter rotating vortex pairs at the downstream that wrinkles the flame front. This counter rotating vortex pairs are the vortex sheet on both sides of the bluff body, which rolls up; hence the induced flow field wraps the flame around these regions of intense vorticity (Fig. 9.15). This wrinkling and corrugation of the flame sheet is caused due to unstable, separated shear layer of the bluff body, also partly due to the flame position which nearly lies parallel to the flow field. As flame generated vorticity (FGV) counterbalances rotating vortex pairs, the wrinkling of flame front is also attenuated and flame front detaches whilst the whole process repeats again. This periodicity of this wrinkling process shows up in Fig. 9.13 (~1s).

![Diagram of vorticity transport equation terms](image)

Figure 9.20: Individual terms of vorticity transport equation (Eq. 9.9) with CH₄: stream lines (purple lines), isotherms (black lines)

Fig. 9.16 shows the upstream flame movement in terms of stream lines and temperature plots during flashback for 30%H₂. Once the flame front is pushed into the mixing tube, the effect of heat-release due to higher combustibility of H₂ mostly drives the further upstream movement. The
Figure 9.21: Stream lines colored with Damköhler (Da) number contours during flashback with 30%H₂: isotherms (black lines)
effects of heat release on the flow field can be understood from the vorticity transport equation (Eq. 9.9) which is written as:

\[
\frac{D\vec{\omega}}{Dt} = \left( \nabla \cdot \vec{u} \right) \vec{\omega} - \left( \vec{\omega} \cdot \nabla \right) \vec{u} - \frac{\nabla \cdot \vec{\nabla} \rho}{\rho^2} + \nu \nabla^2 \vec{\omega} \tag{9.9}
\]

where the RHS terms are: (I) Vortex stretching, (II) Gas expansion, (III) Baroclinic production, and (IV) Viscous diffusion. This equation essentially explains the evolution of the vorticity of a moving fluid element in space. The terms (I) and (IV) have influence regardless of reacting or non-reacting flows. The term (IV) sharply rises across the flame due to change in temperature, and thus enhances the rate of diffusion and dampens the vorticity (Fig. 9.19). However, the misalignment of the pressure and density gradients due to inclination and expansion of the flame with respect to the flow field contributes to the baroclinic production (III) of vorticity (Fig. 9.18). The gas expansion term (II) acts as a sink in reacting cases due to negative sign in the transport equation. This term is directly proportional to the gas dilatation ratio across the flame \((\rho_u/\rho_b)\), which increases as the temperature increases in presence of combustion. These two terms (II & IV) stabilize each other influences (Fig. 9.19). Hence, the net negative azimuthal vorticity is produced (Fig. 9.19) inner edge of the flame (burnt region along the pipe wall) and also along the flame surface, due to interaction between shear generated vorticity and flame generated, baroclinic vorticity.

It is noteworthy that the negative azimuthal vorticity induces the axial velocity to against the main flow direction. The reason behind this is that any velocity field can be broken into an irrotational and rotational part,

\[
\vec{u}(\vec{x}) = \vec{u}_i(\vec{x}) + \vec{u}_r(\vec{x}) \tag{9.10}
\]

where the irrotational part contains no vorticity, \(\nabla \times \vec{u}_i = 0\), and the rotational velocity is given by,

\[
\vec{u}_r(\vec{x}) = -\frac{1}{4\pi} \int \frac{s \times \vec{\omega}(\vec{x}')}{s^3} dV \tag{9.11}
\]
where $\vec{s} = \vec{x} - \vec{x}'$. In vortex breakdown, the axial velocity near the axis stagnates and reverses. The stagnation of core flow is primarily due to the rotational velocity, $\vec{u}_r$ (Darmofal, 1993). Assuming axisymmetric flow, at $r = 0$, the induced velocity due to negative azimuthal velocity as given by Eq. (9.11) simplifies to:

$$w_{ind}(x) = \frac{1}{2} \int_{-\infty}^{\infty} \int_{0}^{\infty} \frac{r'^2 \omega_{\phi}(r', x')}{r'^2 + (x - x')^2} dr'dx'$$  \hspace{1cm} (9.12)

This states that the greater the vorticity, the greater is the induced velocity. Thus, this induced negative velocity pushes the stagnation point ahead of the flame tip (Fig. 9.16, t=8s–t=10.5s) further upstream and helps to form a small recirculation bubble ahead of the flame tip. Fig. 9.16 clearly exhibits the formation of such bubble from t=10.5s to t=12.0s. This fact can also be correlated with the pressure jump observed upstream and across the flame front due to convex flame orientation to the flow field (Fig. 9.18). As observed in Fig. 9.16 the flame front starts interacting with the cross-flow fuel injection as the flame tip starts pushing the upstream stagnation point and forms the small recirculation bubble ahead of it (t=10.5s & t=12.0 s, Fig. 9.16). The formation of this small recirculation bubble ahead of the flame tip gives rise to the generation of greater negative azimuthal vorticity, which in turn, produces higher induced negative velocity and the flame tip movement to further upstream becomes completely uncontrollable. That’s why 30%H₂ exhibits flashback while CH₄ does not show any flashback behavior (Fig. 9.17).

A more detailed observation of vorticity budget terms (Eq. 9.9) supports the above phenomena, which contributes to the generation of negative azimuthal vorticity, in turn produces the induced negative velocity. Fig. 9.19 shows the distribution of change in budget terms between t=8s to t=12.0s for 30%H₂ mixture. The upstream propagation of the flame front is due to increase of the induced negative velocity (Eq. 9.12). A thorough analysis clearly exhibits that the combined effects of vortex stretching and baroclinic production give rise to the negative azimuthal vorticity particularly along the flame front, while the vortex expansion and diffusion terms stabilize.
each other influences. Since negative azimuthal vorticity induces negative axial velocity, vortex stretching and baroclinic production are primarily responsible for upstream flame propagation and leading to flashback. Whereas for CH₄ (Fig.9.20), baroclinic production and vortex stretching contribute to the production of positive azimuthal vorticity along the flame front and that’s why flame front is pushed backed as shown in Fig. 9.20; never leads to flashback and produces quasi stable back-n-forth movement of flame front for this case.

Figure 9.21 show the distribution of Damköhler number (Da) superimposed with the stream lines and isotherms. It represents turbulence-chemistry interaction during flashback. The definition of Da used here to generate these plots is slightly different than Eq. (4.7). The definition used here as follows:

$$Da = \frac{\tau_{mix}}{\tau_{rea}}$$  \hspace{1cm} (9.13)

where $\tau_{mix}$ = mixing time, also referred to as residence tome, flow time, and fluid motion time, $\tau_{rea}$ = reaction time.

$$\tau_{mix} = \frac{Characteristics\ diamter(D)}{inlet\ bulk\ velocity(U_0)}$$  \hspace{1cm} (9.14)

$$\tau_{rea} = \frac{la\ min\ ar\ flame\ thickness(\delta_L)}{la\ min\ ar\ flame\ speed(S_L)}$$  \hspace{1cm} (9.15)

The laminar flame thickness is given by the ratio of the thermal diffusivity to the laminar flame speed ($\delta_L = \alpha/S_L$). Combining all of these equations, the general form of $Da$ becomes

$$Da = \frac{\tau_{mix}}{\tau_{rea}} = \frac{DS_L^2}{U_0\alpha}$$  \hspace{1cm} (9.16)

As observed in the plots (Fig. 9.21), the region of small $Da$ corresponds to the quenching of the reaction, while the regions with large $Da$ correspond to the fast chemical reaction time that prevents local quenching. All the plots in Fig. 9.21 show regions with low $Da$ in the burnt region (inside the flame front) as well as along the reaction zone of flame front. Also, this low $Da$ region increases as the flame tip moves upstream, including radial broadening of reaction zone. In the
stable flame condition at t=8s (Fig. 9.21) the smaller quenching zone (small Da region) does not produce sufficient negative azimuthal vorticity to favor upstream propagation of the flame front. However, when the flame front is pushed further upstream due to recirculation bubble, the stronger quenching (larger region of small Da) gives rise to the production of sufficient negative vorticity, which favors upstream flame propagation during flashback.

In summary, the basic idea of this CIVB is that the flame contributes to vortex breakdown, and results a low or negative flow region ahead of it (recirculation bubble formation with a stagnation point). As the flame tip moves forward, causing the vortex location breakdown region to advance further upstream. This process continues as the flame proceeds further and further upstream. It has been also reported that in CIVB, flashback can occur even if \( S_T \) is everywhere less than the flow velocity (Lieuwen et al., 2008).

9.3 Conclusions

LES with a TF model is used to investigate hydrogen enriched premixed flames in a laboratory based model combustor. The effect of hydrogen addition is mainly studied, especially in the context flame flashback. Upstream flame propagation driven by Combustion Induced Vortex Breakdown (CIVB) is known to be a severe problem for premixed swirl burners, and has been investigated in great details. A CIVB driven flame flashback for a center-body stabilized swirled burner is investigated and reported here on the basis of the of the source terms of the vorticity transport equations. A 2-step chemical scheme for methane combustion and 1-step for hydrogen combustion are invoked to represent the flame chemistry for methane-hydrogen-air combustion. The equivalence ratio for the flame is 0.7 and the geometric swirl number for the configuration is 0.82. This study leads to the following conclusions:

(a) LES-TF model is able to properly capture hydrogen enriched combustion behavior.

(b) Both the reacting and non-reacting velocity profiles are well predicted.

(c) Hydrogen enrichment reduces the size and shape of the recirculation bubble.
(d) Hydrogen enrichment also leads to flame flashback due to higher combustibility.

(e) CIVB driven flame propagation is driving mechanism even for a center-body stabilized swirled burner.

(f) The flame changes the vorticity of the flow field due to its gas-expansion and baroclinic production.

(g) CIVB driven flashback is governed by the interaction of turbulence and the chemistry due to its influence on the vorticity.

(h) The vortex stretching and baroclinic production contribute to the net vorticity generation leading to the occurrence of CIVB driven flashback which produces considerable levels of negative axial velocity that favors upstream flame propagation.

(i) If the flame does not produce enough baroclinic torque, then the combined effects of gas-expansion and diffusion can stabilize the vortex flow and prevent flashback. What exactly happens in the case of CH₄.

(j) Since the previous studies (Noble et al., 2006; Nauert et al., 2007; Knole et al., 2009) on different swirl stabilized burner reported CIVB driven flashback, and the present study with center-body stabilized swirled burner reveals the same fact; there is evidence that the observed effects can be considered as a prevailing flashback mechanism in swirled premixed burners.

This study demonstrates that the Thickened-Flame based LES approach with simplified chemistry for reacting flows is a promising tool to investigate reacting flows in complex geometries.
Chapter 10 Flashback in Hydrogen Enriched Premixed Combustion: Effects of Swirl, Geometry and Premixedness

The current trend in the development of modern gas turbine combustor is to operate under lean conditions to reduce emissions. This can be best achieved by making the design more compact with low surface to volume ratio while maintaining the higher turbine inlet temperature. The compact design requires efficient mixing together with a compact premixed flame. A conceptual design may consist of a primary fuel injector nozzle, within which air passes through a swirler arrangement to properly mix the fuel with the incoming air. The turbulent swirling premixed fuel-air jet together with sudden expansion to the full combustor chamber provide an efficient way of improving mixing and help in stabilizing the flame. Hence due to the performance requirements, there is considerable interest in identifying the optimal swirl and geometric conditions to achieve specific practical goals.

One of the widely used techniques is jet-in-cross flow fuel injection systems due to its effectiveness and simplicity. The degree and rate of the mixing process is especially important in combustion applications. Boutazakhti et al. (2001) studied the effect of jet mixing to improve the understanding of the relationship between mixing, chemical kinetics, and combustion efficiency for air jets in a hot reacting cross-flow. Other parameters such as the residence time and the equivalence ratio (Rizk and Mongia, 1993; Zelina and Ballal, 1997) are equally important factors affecting combustion efficiency of air jets in a reacting cross-flow.

The other key factor in premixed combustion systems is Swirl. Swirl has great impact on the performance of gas turbine combustors including fuel-air pre-mixedness. Swirl is usually used to obtain high mixing rates as well as to stabilize the flames. Generally, the swirling motion at the inlet is generated using some kind of guide vanes, inlet tangential flow injections or by other means. When the strength of the swirl becomes high enough, it leads to formation of
internal recirculation zone (IRZ), which is known as vortex breakdown phenomenon in fluid mechanics. Especially in LP combustion, IRZ plays an important role by holding the hot combustion products and radicals as well as enhance the flame anchoring to the recirculation zone. However in the non-premixed combustion, IRZ usually enhances fuel/air mixing of fuel and intensity of combustion as well. Moreover, it has important influence on the flame shape, flame stability and heat release rate, as well as on emission. An extensive review on swirling flows can be found in (Syred and Beer, 1974; Lucca-Negro et al., 2001; De et al., 2009). Tangirala et al. (1987) studied a non-premixed swirl burner where they reported that the mixing and flame stability can be improved with swirl upto a swirl number of about unity, beyond which a further increase in swirl reduces the turbulence level as well as the flame stability. Broda et al (1998) and Seo (1999) experimentally investigated the combustion dynamics in a lean-premixed swirl stabilized combustor. One of the key influences of the swirl on the flow field is the formation of the recirculation zone at the burner exit. As the swirl number exceeds a critical value, vortex breakdown takes place and leads to the formation of an internal recirculation zone (Huang and Yang, 2005). This recirculation not only enhances fuel-air mixing, but also carries hot products back to the reactants and plays an important role in the flame holding. However, despite several years of research, the mechanisms of vortex breakdown are only partially understood (Lucca-Negro et al., 2001; Syred, 2006; Duwig et al., 2007). Recently, a number of studies have analyzed swirling flames using numerical approaches and experimental techniques as well (De et al., 2009).

Recently, hydrogen enrichment has been found to be a promising approach of increasing the LBO limits of hydrocarbon fuels, thereby can provide stable combustion at lean mixture conditions (Griebel et al., 2007). Hence the problem of flame holding at LP conditions can be avoided by increasing the hydrogen proportion in the fuel. Increase in hydrogen proportion
will assure better flame stability but, at the very same time, it will make the combustor more susceptible to flashback. Thus flashback becomes an inherent problem in this type of system due to addition of hydrogen, since hydrogen flame speeds are quite high (Mariotti et al., 2002). It is an intrinsic behavior of premixed systems as the flame stabilizes at upstream of the combustion chamber. Flashback has been extensively investigated by several researchers (Wohl, 1952; Plee et al., 1978; Putaam et al., 1948) and they reported that the complexity of the topic becomes more substantial in swirling flows (Noble et al., 2006). There are several explanations found in the literature (Fritz et al, 2004; Kröner et al, 2003; Kiesewetter et al., 2003), but the occurrence of flashback is unique to each system. Flashback may occur due to different reasons as: (a) Flashback by flame propagation, (b) Flashback in boundary layers, (c) Flashback due to turbulent flame speed, (d) Flashback due to combustion instabilities, and (d) Flashback due to vortex breakdown. Among all of these, flashback in strongly swirled flow mostly occurs either due to combustion instabilities or vortex breakdown. Although swirled burners being more sensitive to combustion instabilities, and may become prone to triggering the flashback in these types of combustors; however, the fluctuations required to cause such problems are beyond the acceptable noise levels in most combustion systems.

Vortex breakdown in swirled burner occurs when the azimuthal velocity becomes larger than the axial velocity. Moreover, this vortex breakdown is often accompanied by a large recirculation zone with high reverse flow velocities in combustions systems, and the reverse velocities can promote upstream flame propagation and flashback is the consequence. The formation of vortex breakdown strongly depends on the geometry, and if the swirl number exceeds a critical value the recirculation zone is able to extend itself throughout the entire mixing section. In isothermal flows, this effect can be prevented by selecting the swirl number; however, the chemical reaction can nevertheless lead to a breakdown of the flow, combined with upstream flame propagation.
This mechanism is called as combustion-induced vortex breakdown (CIVB) as reported by Fritz et al. (2004), Sommerer et al. (2004). Normally, swirled burner and swirl stabilized flame without center-body are more susceptible to this kind of problem. Recent studies by Nauert et al. (2007), Kiesewetter et al. (2007), Kröner et al. (2003, 2007), Knole et al. (2008), Konle and Sattelmayer (2009), Voigt et al. (2009) also reported this CIVB driven flashback in swirled burner.

![Graphs showing U/U_0 and W/U_0 with r/2D as a variable at X/2D = 0.79 and X/2D = 1.58](image)

Figure 10.1: Non-reacting flow results for Re=13339 at different axial locations [D=Center-body diameter]: Experimental data (Δ), Lines are LES predictions: fine mesh (—, blue solid lines), coarse mesh (- - - , purple dashed lines). Mean axial velocity U/U_0, Mean tangential velocity W/U_0, Axial velocity fluctuation u_rms/U_0, Tangential velocity fluctuation w_rms/U_0.

Flashback into the pre-mixer section leads to thermal overload and destruction of the hardware therefore it must be avoided at all load conditions (Kiesewetter et al., 2007). Flashback can be prevented by using specially designed flame holders or by injecting syngas in a separate non-premixed arrangement. However, in transitioning from natural gas as the fuel of choice to syngas, it is desirable to keep hardware changes to a minimum, given the extensive body of knowledge with current natural gas related hardware. Several studies have investigated premixed
flames of H\textsubscript{2}-hydrocarbon fuel mixtures in swirled burner. Schefer (2003) and Schefer et al. (2002) studied the effects of hydrogen injection in methane/air flames in a completely premixed mode combustor at atmospheric pressure and swirling conditions. They reported that the addition of H\textsubscript{2} to methane (CH\textsubscript{4}) fuel decreases the adiabatic flame temperature at LBO and, hence, decreases the CO emissions (without effecting the NOx emissions). The H\textsubscript{2}-enriched CH\textsubscript{4} flame produces shorter flames with more intense reaction zones. Gupta et al. (1998, 2001) investigated the effects of swirl on combustion characteristics of premixed flames. Kröner et al. (2003, 2007) also reported flashback due to combustion induced vortex breakdown (CIVB) in swirling flows for different CH\textsubscript{4}+H\textsubscript{2} mixtures. They reported that the CIVB happened to be the prevailing mechanism in a swirled burner without center-body. Strakey et al. (2007) in their study investigated the effects of hydrogen addition on lean extinction in a swirl stabilized combustor. They reported the lean blowout limits for methane/hydrogen mixtures at pressures ranging from 1 to 8 atmospheres. More recently, Kim et al. (2009) reported the effects of H\textsubscript{2} addition in a confined and unconfined swirl burner operating at lean conditions through PIV diagnostics. They clearly showed the impact of hydrogen on flame structure and flow filed including the pollutant emissions. They also reported the effects of swirl intensity on hydrogen enriched flame how that alters the flow field. Tuncer et al. (2009) also investigated dynamics, NOx and flashback characteristics in a confined premixed hydrogen-enriched methane flames for a laboratory scale swirled combustor. Ballester et al. (2009) also carried out chemoluminescence measurements to study premixed natural gas flames with hydrogen blending for a swirl-stabilized combustor.

In this work, a Thickened Flame (TF) model (Colin et al., 2000) is used where the flame is artificially thickened to resolve it on computational grid points where reaction rates from kinetic models are specified using reduced mechanisms. The influence of turbulence is represented by a parameterized efficiency function. A key advantage of the TF model is that it directly solves the
species transport equations and uses the Arrhenius formulation for the evaluation of the reaction rates.

In turbulent premixed combustion, a popular approach is to rely on the flamelet concept, which essentially assumes the reaction layer thickness to be smaller than the smallest turbulence scales. The two most popular model based on this concept are the flame surface density model (FSD) (Hawkes and Cant, 2001) and the G-equation model (Williams, 1985; Peters, 2000). It has been reported that the FSD model is not adequate beyond the corrugated flamelet regime (Düsing et al., 2006; Pitsch et al., 2002), while the G-equation approach depends on a calculated signed-distance function that represents an inherent drawback of this method.

Another family of models relies on the probability density function (PDF) approach (Poper, 1985). This is a stochastic method, which directly considers the probability distribution of the relevant stochastic quantities in a turbulent reacting flow. The PDF description of turbulent reacting flow has certain theoretical benefits; the complex chemistry is taken care of without applying any ad-hoc assumptions (like 'flamelet' or 'fast reaction'). Moreover, it can be applied to non-premixed, premixed, and partially premixed flames without having much difficulty. However, the major drawback of the PDF transport approach is its high dimensionality, which essentially makes the implementation of this approach to different numerical techniques, like FVM (Finite Volume Method) or FEM (Finite Element Method), limited.

The major advantage associated with this TF model is the ability to capture the complex swirl stabilized flame behavior which is often found in a gas turbine combustor. Since this type of geometry with the premixing section does not guarantee a perfectly premixed gas at the dump plane, the fully premixed assumption in the numerical model is not valid any more. The present TF model is capable of taking care of this type of partially premixed gas since we solve for the individual species transport equations and the reaction rates are specified using Arrhenius
expressions.

The configuration of interest in the present work is an unconfined swirl-stabilized flame. In this investigation, we investigate flashback behavior of hydrogen enriched premixed swirl-stabilized flames. The goal of this study is to analyze the flow and combustion physics in hydrogen enriched premixed flame and, in particular, to explore how swirl, premixednes and geometry play a role in the flame flashback behavior.

10.1 Flow Configuration and Numerical Details

The configuration considered here is an unconfined swirl burner as shown in Fig. 9.1. The 45° swirl vane is fitted with a solid center body which also acts as a fuel injector. This center body extends beyond the swirl vane and is flush with the dump plane of the combustor. The diameter of the center body is 12.7mm (0.5 inch) and the O.D. of the swirler is 34.9 mm (1.375 inch). Methane and hydrogen gas is injected radially from the center body through eight holes immediately downstream of the swirler vane. The fuel/air mixer is assumed to be perfectly premixed at the dump plane and the equivalence ratio is calculated to be $\phi=0.7$. The investigation is carried out for Reynolds number, $Re=13339$ (based on inlet bulk velocity and hydraulic diameter) at atmospheric pressure and temperature with 30%H2 mixture. The swirl number, defined as the ratio of the axial flux of the tangential momentum to the product of axial momentum flux and a characteristic radius, used for this investigation are $S=0.38$, 0.82 and 1.76.

In this investigation, the computational method uses LES combined with a TF approach for combustion. To model the turbulent flow, LES is used where the energetic larger-scale motions are resolved, and the small scale fluctuations are modeled. Therefore, the equations solved are the filtered governing equations for the conservation of mass, momentum, energy and species transport in a curvilinear coordinate system. The sub-grid stress modeling uses a dynamic Smagorinsky model. Modeling the flame-turbulence interaction in premixed flames requires tracking of the thin flame front on the computational grid. Hence, we use the thickened flame
approach which is a cost-effective strategy while allowing the chemistry to be represented. In this technique, the flame front is artificially thickened to resolve it on the computational grid while allowing the flame to propagate at the same speed as the un-thickened flame. The artificial thickening of the flame front is obtained by multiplying the diffusion term by a factor F and dividing the reaction rates by the same factor to maintain the flame speed. More detailed description of this technique is found in the literature (Chapter 4). The major advantage associated with this TF model is the ability to capture the complex swirl stabilized flame behavior which is often found in a gas turbine combustor. Since this type of geometry with the premixing section does not guarantee a perfectly premixed gas at the dump plane, the fully premixed assumption in the numerical model is not valid any more. The present TF model is capable of taking care of this type of partially premixed gas since we solve for the individual species transport equations and the reaction rates are specified using Arrhenius expressions.

Detailed description on computational domain, chemistry model and boundary conditions can be found under the subsection 'Numerical details (9.1.1)' of previous chapter (Chapter 9).

10.2 Results and Discussion

We will first report the non-reacting LES calculations to ensure that the grid and boundary conditions are properly chosen, and to assess the cold-flow flow characteristics. This will be followed by a discussion of the hydrogen enriched flow calculations where we will examine flashback behavior and analyze how swirl, geometry and premixedness influence this behavior.

10.2.1 Non-reacting Flow Results

Figure 10.1 shows the radial distribution of axial and tangential mean velocity profiles, axial and tangential velocity fluctuations at different axial locations for Re=13339. In general, LES and the experimental data for radial distribution of the axial and tangential mean velocity profiles, and the axial and tangential fluctuations at different axial locations are found to be in good agreement. It is observed that the shape, size, and the intensity of the recirculation zone (region of
negative axial velocities at the center) are well predicted along with the overall spreading of the turbulent swirling jet. Also, the RMS fluctuations of the axial and tangential velocities are in good agreement with the experimental data. The peak in the axial velocity fluctuations is observed to be in the shear layer and between the location of the peak velocity and the recirculation bubble. In this region, the steepest velocity gradient $\partial U_i/\partial x_j$ is obtained and promotes the production of the peak kinetic energy. The tangential velocity fluctuations show a flatter profile than the axial velocity fluctuations and their peaks are shifted radially inwards as for the mean tangential velocities. Since the fine mesh (3.94M grid points) results are found to be in better agreement with the experimental data, this fine mesh is chosen for reacting flow calculations. More detailed discussion on non-reacting flow results can be found in the literature by De et al. (2009).

10.2.2 Reacting Flow Results

In this section we will present all the reacting flow calculations for $\text{Re}=13339$ with 30\%H$_2$ mixture.

10.2.2.1 Effects of Swirl

Here the flow configuration has jet-in-cross flow fuel injection system. Means, the fuel is injected right after the step (Fig. 9.3) and the inlet swirled air is mixed with the injected fuel to have a premixed mixture at dump plane.

Figure 10.2 shows stream line contours superimposed with normalized axial velocity at different swirl strength ($S=0.38$, $S=0.82$, $S=1.76$) for $\text{Re}=13339$ with 30\%H$_2$. Usually, the swirl enhances fuel-air mixing to achieve premixed mixture at the dump plane of combustor chamber. Increasing swirl strength increases the mixing, at the same time increases the turbulence level as well. The effect of different swirl strength is clearly observed in axial velocity profiles. As observed the magnitude of the peak axial velocity increases by $\sim$8\% ($S=0.38$-$S=0.82$) and $\sim$30\% ($S=0.38$-$S=1.76$) with the increase in swirl strength. As the higher swirl produces more turbulence, which, in turn increases the heat release due to higher turbulence-chemistry interaction; hence
Figure 10.2: Time averaged stream line contours at different $S$
Figure 10.3: Recirculation bubble size for different $S$

Figure 10.4: Reacting flow results for $S=0.82$ at different axial locations: Experimental data ($\Delta$), Lines are LES predictions: Mean axial velocity $U/U_\infty$, Axial velocity fluctuation $u_{rms}/U_\infty$
Figure 10.5: Time averaged temperature contours (K scale) at different S
Figure 10.6: Instantaneous flame propagation for different S (Temperature in K scale)
flame temperature increases and peak density decreases by \( \sim 11\% (S=0.38-S=0.82) \) and \( \sim 28\% (S=0.38-S=1.76) \). Thus flow accelerates more along the flame front and exhibit higher magnitude. However, at a fixed hydrogen mixture (30%H\(_2\)), the increase in swirl strength increases the size of the recirculation bubble (shown in Fig. 10.3), thus the overall recirculation flow increases. As observed the width of the recirculation zone is also broadened due to higher centrifugal force at higher swirl strength (Figs. 10.2 & 10.3). Similar trend is also reported in the literature by Kim et al. (2009).

The radial distributions of mean axial velocity and axial velocity fluctuations are shown in Fig. 10.4 for \( S=0.82 \). The overall agreement of the predictions with the data is found to be quite reasonable, considering the complexity of the physical processes and the configuration. With increasing axial distance the magnitude of the peak velocity decreases and the location of the peak is moved further outwards radially. While the general agreement between the data and predictions are satisfactory, and the LES results show the right qualitative features and the peak magnitudes, there are intrinsic differences between the predictions and data. The behavior of predicted RMS fluctuations can be associated with the higher temperature in the product region (Fig. 10.5). This corresponds to the burnt and un-burnt regions in the inner part of the shear layer and associated with the high velocity gradients where the turbulence production due to the mean velocity gradient is the highest. The lower magnitude is located in the burnt region of the shear layer downstream of the center body where the temperatures are higher. The high temperatures cause the viscosity value to go up, and this reduces the magnitude of the peak stress component. The higher magnitude is observed in the un-burnt regions of the shear layer where the temperatures are relatively on the lower side which reduces the viscosity value and in turn exhibits higher fluctuating components. Similar trends for RMS fluctuations have also reported by other researchers reporting calculations (Galpin et al., 2008).
Figure 10.5 shows the time-averaged temperature profiles at different swirl strength. As observed flame flashback occurs at higher $S$ and the flame moves upstream of the dump plane to premixing section and stabilizes there. This can be related to the high level of turbulence generated at higher swirl in addition to the higher low velocity region along the wall of the center-body. Higher turbulence-chemistry interaction increases heat release production, especially in $H_2$ enriched mixture, and promotes flame flashback. The detailed discussion on flashback is provided in the following section.

Figure 10.6 shows the instantaneous temperature plots for different $S$. It shows how the flame starts propagating upstream and then stabilizes in the mixing tube, especially at higher swirl strength, i.e. $S=0.82$ and $S=1.76$. For $S=0.38$, the flame front also moves little bit upstream of the dump plane but does not move further upstream as observed in Fig. 10.6. Upstream flame propagation, usually characterized as flame flashback, occurs when the burning velocity exceeds the local flow velocity. In the present case, the flash back is initiated due to Combustion Induced Vortex Breakdown (CIVB) and then accompanied with the favorable condition, due, in part, low velocity in B/L and higher local burning velocity. As the flame starts moving upstream, especially for $S=0.82$ and $S=1.76$, it encounters fuel rich region due to the fuel injection point, and that induces higher flame propagation velocity in presence of highly combustible $H_2$. More often, the CIVB refers to the vortex break down due to chemical reaction which becomes more intensive in presence of $H_2$ and turbulence, enhanced at higher swirl strength as well. Additionally, this vortex breakdown is often accompanied by a large recirculation zone with high reverse flow velocities in combustions systems, and the reverse velocities can promote upstream flame propagation and flashback is the consequence (Fig. 10.6).

It is to be noted that the formation of recirculation zone is the consequence of vortex breakdown. Usually, the recirculation bubbles bring the heat and reactive species back to the flame
Figure 10.7: Stream lines colored with temperature contours (K scale) for S=0.38: no flashback: isotherms in black lines (300, 675, 1050, 1425 K)
Figure 10.8: Stream lines colored with temperature contours (K scale) for $S=0.82$ during flashback: isotherms in black lines
Figure 10.9: Stream lines colored with temperature contours (K scale) for S=1.76 during flashback: isotherms in black lines
tip and provides flame-holding at the dump plane. However, the recirculation zone gives rise to the azimuthal vorticity component in this region and that produces positive or negative induced velocity following the Bio-Savart law, as give by Eq. 10.4 (Kiesewetter et al., 2007; Knole et al., 2008) depending on the sign of azimuthal vorticity. The position and motion of this recirculation bubble largely depends on the balance maintained between the induced velocity and irrotational axial velocity. Slight changes in the flow field can alter this balance and result in the upstream movement of the recirculation bubble. This unsteady motion of recirculation bubble actually promotes the upstream flame propagation in the mixing tube, and thereafter it is accompanied by the higher induced negative velocity due to production of negative azimuthal vorticity. As observed for S=0.38 in Fig. 10.7, the flame front moves little bit upstream into the mixing tube and tends to interact with the fuel injection system (Fig. 10.7) and form a small recirculation bubble ahead of flame front at t=9.2s (Fig. 10.7). Since the further upstream movement of the flame front is annihilated due to unfavorable condition, the flame front is actually pushed back by the incoming flow (t=11.2s & t=17.6s in Fig. 10.7) and the formed small recirculation bubble (t=9.2s & t=14.2 s in Fig. 10.7) also disappears at t=11.2s & t=17.6s (Fig. 10.7). This back-n-forth interaction of flame front and incoming flow maintains a balance between flow field and flame front without occurrence of flashback at lower swirl strength. That’s why the upstream flame propagation in this case is not observed.

However, at higher swirl strength S=0.82 & S=1.76 case, the upstream flame movement is initiated due to unsteady motion of recirculation bubble, formed due to vortex breakdown. Fig. 10.8 and 10.9 depict the time instant snap shots of stream lines superimposed with temperature contours during upstream flame propagation for S=0.82 and S=1.76, respectively. As observed in Fig. 10.8 for S=0.82, the flame front is nicely stable close to the dump plane at t=9s and there is no interaction between flame front and jet-in-cross flow fuel injection. As the flame front moves
Figure 10.10: Individual terms of vorticity transport equation (Eq. 10.1) for $S=0.38$: no flashback: isotherms in black lines
Figure 10.11: Individual terms of vorticity transport equation (Eq. 10.1) for S=0.82 during flashback: isotherms in black lines
Figure 10.12: Individual terms of vorticity transport equation (Eq. 10.1) for S=1.76 during flashback: isotherms in black lines
further upstream at t=12.2s due to upstream movement of stagnation point (formed due to vortex breakdown), it starts interacting with the fuel injection system due to increase in pressure ahead of flame front. The pressure difference between upstream and downstream of flame front causes the formation of a small recirculation bubble ahead of flame front and also forms a local stagnation point ahead of flame tip, which becomes more prominent later time instant at t=14.2s (Fig. 10.8). The formation of this small recirculation bubble ahead of the flame tip gives rise to the generation of greater negative azimuthal vorticity, which in turn, produces higher induced negative velocity and the flame tip movement to further upstream becomes completely uncontrollable. That’s why this case exhibits flashback while S=0.38 case does not show any flashback behavior (Fig. 10.7). At S=1.76 (Fig. 10.9) compared to S=0.82 case (Fig. 10.8), the flame is already moved deep into upstream mixing tube at the earlier time instant of t=7.6s (Fig. 10.9) including distinct formation of two recirculation bubbles. One recirculation bubble, formed due to vortex breakdown, pushes the flame front upstream and then as the flame front moves further upstream it starts interacting with the fuel injection system and forms another recirculation bubble ahead of flame tip. This gives rise to the production of higher induced negative velocity that promotes upstream flame propagation aggressively at higher swirl strength (S=1.76). At t=9.2s in Fig. 10.9, the flame front already reaches the fuel-injection system. The observation in Figs. 10.7-10.9 confirms that the upstream flame propagation becomes favorable with the increase in swirl strength. The formation of this recirculation bubble due to vortex breakdown can also be attributed to the shear layer instability (KH instability) where the vorticity is continuously generated at the bluff body, convected downstream, and lead to vortex roll up and pairing. Once the flame front is pushed into the mixing tube, the effect of heat-release due to higher S including highly combustible H₂ mostly drives the further upstream movement. The effects of heat release on the flow field can be
understood from the vorticity transport equation (Eq. 10.1) which is written as:

\[
\frac{D \vec{\omega}}{Dt} = \left( \vec{\omega} \cdot \nabla \right) \vec{u} - \vec{\omega} \left( \nabla \cdot \vec{u} \right) - \frac{\nabla p \times \nabla \rho}{\rho^2} + \nu \nabla^2 \vec{\omega} \\
\tag{10.1}
\]

where the RHS terms are: (I) Vortex stretching, (II) Gas expansion, (III) Baroclinic production, and (IV) Viscous diffusion. This equation essentially explains the evolution of the vorticity of a moving fluid element in space. The terms (I) and (IV) have influence regardless of reacting or non-reacting flows. The term (IV) sharply rises across the flame due to change in temperature, and thus enhances the rate of diffusion and dampens the vorticity (Figs. 10.10 - 10.12). However, the misalignment of the pressure and density gradients due to inclination and expansion of the flame with respect to the flow field contributes to the baroclinic production (III) of vorticity (Fig. ??). The gas expansion term (II) acts as a sink in reacting cases due to negative sign in the transport equation. This term is directly proportional to the gas dilatation ratio across the flame ($\rho_a/\rho_b$), which increases as the temperature increases in presence of combustion. These two terms (II & IV) stabilize each other influences (Figs. 10.10-10.12). Hence, the negative aximuthal vorticity is produced (Figs. 10.10 - 10.12) inner edge of the flame (burnt region along the pipe wall) and also along the flame surface, due to interaction between shear generated vorticity and flame generated, baroclinic vorticity. While for $S=0.38$ (Fig. 10.10), sufficient negative azimuthal vorticity is not produced along the flame front which can help the upstream flame propagation and makes this case stable without showing any flashback. In fact for this case, the baroclinic production gives rise to positive azimuthal vorticity and pushes back the flame front by generating positive induced velocity, whereas in the case of $S=0.82$ (Fig. 10.11) baroclinic production is accompanied by the stretching term and both these terms give rise to the production of sufficient negative azimuthal vorticity that promotes upstream flame propagation. For $S=1.76$ (Fig. 10.12) compared to $S=0.82$, this effect is very dominant and aggressively favors the upstream flame movement.

In general, the negative azimuthal vorticity induces the axial velocity to against the main flow
direction. The reason behind this is that any velocity field can be broken into an irrotational and rotational part,

\[ \overrightarrow{u}(\overrightarrow{x}) = \overrightarrow{u}_i(\overrightarrow{x}) + \overrightarrow{u}_r(\overrightarrow{x}) \quad (10.2) \]

where the irrotational part contains no vorticity, \( \nabla \times \overrightarrow{u}_i = 0 \), and the rotational velocity is given by,

\[ \overrightarrow{u}_r(\overrightarrow{x}) = -\frac{1}{4\pi} \int \frac{\overrightarrow{s} \times \overrightarrow{\omega}(\overrightarrow{x}')}{s^3} dV \quad (10.3) \]

where \( \overrightarrow{s} = \overrightarrow{x} - \overrightarrow{x}' \). In vortex breakdown, the axial velocity near the axis stagnates and reverses. The stagnation of core flow is primarily due to the rotational velocity, \( \overrightarrow{u}_r \) (Darmofal, 1993). Assuming axisymmetric flow, at \( r = 0 \), the induced velocity due to negative azimuthal velocity as given by Eq. (10.3) simplifies to:

\[ w_{ind}(x) = \frac{1}{2} \int_{-\infty}^{\infty} \int_{0}^{\infty} \frac{r'^2 \omega_p(r', x')}{[r'^2 + (x - x')^2]^{3/2}} dr' dx' \quad (10.4) \]

This states that the greater the vorticity, the greater is the induced velocity. Thus, the negative induced velocity pushes the stagnation point ahead of the flame tip (Fig. 10.7-10.9) further upstream and results in production of higher negative azimuthal vorticity. This fact can also be correlated with the pressure jump at upstream and across the flame front due to convex flame orientation to the flow field. Also, the observation in Fig. 10.7 clearly shows that there is no interaction of flame tip with the cross-flow fuel injection at S=0.38 case. However, it starts interacting with the cross-flow fuel injection as the flame tip starts pushing the upstream stagnation point in the case of higher swirl S=0.82 and S=1.76 (Figs. 10.8- 10.9). This complex interaction at the flame tip gives rise to the generation of greater negative azimuthal vorticity, which in turn, produces higher induced velocity and the flame tip movement to further upstream becomes completely uncontrollable at higher swirl strength, i.e. S=0.82 and S=1.76.

A more detailed observation of vorticity budget terms (Eq. 10.1) supports the above phenomena, which contributes to the generation of negative azimuthal vorticity, in turn produces
the induced negative velocity. Figures 10.11 & 10.12 show the distribution of change in budget terms for S=0.82 (between t=9.0s and t=12.2s) and S=1.76 (between t=7.6s and t=9.2s), respectively. The upstream propagation of the flame front is due to increase of the induced negative velocity (Eq. 10.4). A thorough analysis clearly exhibits that the combined effects of vortex stretching and baroclinic production give rise to the negative azimuthal vorticity particularly along the flame front, while the vortex expansion and diffusion terms stabilize each other influences. Since negative azimuthal vorticity induces negative axial velocity, vortex stretching and baroclinic production are primarily responsible for upstream flame propagation and leading to flashback at higher swirl strength (S=0.82 & S=1.76). Moreover, Figs. 10.8- 10.9 also support this fact that the flame tip encounters much higher negative induced velocity in between t=12.2s & t=9.0s for S=0.82 and t=7.6s & t=9.2s for S=1.76 due to combined effect of vortex-stretching and baroclinic production and that increases consistently. Whereas for S=0.38 (Fig. 10.10), baroclinic production contributes to the production of positive azimuthal vorticity along the flame front and that’s why flame front is pushed backed as shown in Fig. 10.10; never leads to flashback and produces stable movement of flame front for this case.

Figure 10.13 shows the distribution of Damköhler number (Da) superimposed with the stream lines and isotherms contours for S=0.38 & 1.76. It represents turbulence-chemistry interaction during flashback. The definition of Da used here to generate these plots is slightly different than Eq. (4.7). The definition used here as follows:

$$Da = \frac{\tau_{mix}}{\tau_{reac}}$$  \hspace{1cm} (10.5)

where \(\tau_{mix}\) = mixing time, also referred to as residence tome, flow time, and fluid motion time, \(\tau_{reac}\) = reaction time.

$$\tau_{mix} = \frac{Characteristics\ diamter(D)}{inlet\ bulk\ velocity(U_o)}$$  \hspace{1cm} (10.6)
Figure 10.13: Stream lines colored with Damköhler (Da) number contours for different S: isotherms (black lines)
Figure 10.14: Time averaged temperature contours (K scale) at $S=0.82$: (a) perfectly premixed inlet, (b) jet-in-cross-flow fuel injection
\[ \tau_{\text{react}} = \frac{\text{laminar flame thickness}(\delta_L)}{\text{laminar flame speed}(S_L)} \]  

The laminar flame thickness is given by the ratio of the thermal diffusivity to the laminar flame speed \((\delta_L = \alpha / S_L)\). Combining all of these equations, the general form of \(Da\) becomes

\[ Da = \frac{\tau_{\text{mix}}}{\tau_{\text{react}}} = \frac{DS_L^2}{U_o \alpha} \]  

As observed in the plots (Fig. 10.13), the region of small \(Da\) corresponds to the quenching of the reaction, while the regions with large \(Da\) correspond to the fast chemical reaction time that prevents local quenching. All the plots in Fig. 10.13 show regions with low \(Da\) in the burnt region (inside the flame front) as well as along the reaction zone of flame front. Also, this low \(Da\) region increases as the flame tip moves upstream, including radial broadening of reaction zone. In the stable flame condition for \(S=0.38\) (\(t=9.2s\)-\(t=17.6s\) in Fig. 10.13) the smaller quenching zone (small \(Da\) region) does not produce sufficient negative azimuthal vorticity to favor upstream propagation of the flame front. However, when the flame front is pushed further upstream due to recirculation bubble for \(S=1.76\), the stronger quenching (larger region of small \(Da\)) gives rise to the production of sufficient negative vorticity, which favors upstream flame propagation during flashback.

**10.2.2.2 Effects of Premixedness**

Here the flow configuration has fixed swirl strength of \(S=0.82\). Once set-up has jet-in-cross flow fuel injection system; means the fuel is injected right after the step (Fig. 9.3) and the inlet swirled air is mixed with the injected fuel to have a premixed mixture at dump plane. Other set-up assumes everything is premixed at the upstream inlet (Fig. 9.3) based on \(\phi=0.7\).

Figure 10.14 shows the time-averaged temperature profiles for different fuel injection system at particular swirl strength. As clearly observed both the systems exhibit flashback and the flame moves upstream of the dump plane to premixing section and stabilizes there. Notably,
Figure 10.15: Instantaneous flame propagation for $S=0.82$: (a) perfectly premixed inlet, (b) jet-in-cross-flow fuel injection (Temperature in K scale)
the setup with perfect premixedness rather shows more susceptible to flashback prone. This is associated with the premixedness of the fuel-air mixture as well as swirl strength that enhances turbulence-chemistry interaction, producing higher heat-release in hydrogen enriched mixture and the flame flashback is the consequence.

Figure 10.15 shows the time series temperature plots for both perfectly premixed inlet and jet-in-cross flow fuel injection systems at $S=0.82$. As observed for perfectly premixed case, the flame front has moved into the mixing tube upto $X/2D=2$ at very earlier instant ($t=9.0s$) due to recirculation bubble movement, while in the other case (jet-in-cross flow) the flame front has only moved upto $X/2D=0.5$ at same time instant. Here, the flash back is initiated due to Combustion Induced Vortex Breakdown (CIVB) and then accompanied with the favorable condition, due, in part, low velocity in B/L and local burning velocity. For perfectly premixed case rich fuel-air mixture in addition to higher turbulence levels ($S=0.82$) induces higher flame propagation velocity compared to other case, and exhibits to be more flashback prone. In addition, this vortex breakdown is often accompanied by a large recirculation zone with high reverse flow velocities in combustions systems, and the reverse velocities can promote upstream flame propagation and flashback is the consequence (Fig. 10.15).

As noted and discussed earlier, the formation of recirculation zone is the consequence of vortex breakdown. In general, the recirculation bubbles bring the heat and reactive species back to the flame tip and provides flame-holding at the dump plane, while giving rise to the azimuthal vorticity component in this region which produces positive or negative induced velocity depending on the sign of azimuthal vorticity. However, the position and motion of this recirculation bubble is very sensitive to the flow field and largely depends on the balance maintained between the induced velocity and irrotational axial velocity. Slight changes in the flow field can alter this balance and result in the upstream movement of the recirculation bubble. This unsteady motion of
Figure 10.16: Stream lines colored with temperature contours (K scale) during flame movement for S=0.82 with perfectly premixed inlet during flashback: isotherms in black lines
Figure 10.17: Mixture fraction ($Z$) contours during flame movement for $S=0.82$ during flashback: (a) perfectly premixed inlet, (b) jet-in-cross-flow fuel injection, isotherms in black lines.
Figure 10.18: Local Flame Index (FI) contours during flame movement for $S=0.82$ during flashback: (a) perfectly premixed inlet, (b) jet-in-cross-flow fuel injection, isotherms in black lines: non-premixed (FI $< 0.0$), premixed (FI $> 0.0$)
recirculation bubble (shown in Fig. 10.16) actually promotes the upstream flame propagation in the mixing tube, and thereafter it is accompanied by the higher negative induced velocity due to production of negative azimuthal vorticity. Formation of such bubble (due to vortex breakdown) is observed for perfectly premixed case in Fig. 10.16, including the movement of the stagnation point (as bubble moves) into the upstream mixing tube at very early time instant (t=9.0s). That’s why the upstream flame propagation in this case does exhibit severely flashback prone compared to the other case (jet-in-cross flow, Fig. 10.8).

Considering the perfectly premixed inlet case, the upstream flame movement is initiated due to upstream propagation of recirculation bubble. Fig. 10.16 shows the time instant snap shots of stream lines superimposed with temperature contours. Compared to jet-in-cross flow case (Fig. 10.15), the flame is already moved deep into upstream mixing tube at the time instant of t=9.0s (Fig. 10.16) including upstream stagnation point along the bluff-body wall. Evidently vortex break down due to chemical reaction (CIVB) is more intensive in this case and thus making this system more susceptible to flashback prone. Due to perfectly premixed inlet, the flame tip encounters much more fuel rich condition compared to jet-in-cross flow configuration, thus enhances chemical reaction. Also, the presence of highly combustible H2 in fuel mixture makes the upstream flame movement much more severe in this case compared to other set up (jet-in-cross flow). Figures 10.17 & 10.18 depict the fuel mixture fraction contours and local Flame Index (FI) contours along the vicinity of flame front during flashback for the different injection systems. Fuel mixture fraction and local FI is calculated based on the following expressions:

\[
Z = \frac{sY_F - Y_O + Y_O^o}{sY_F + Y_O^o}
\]  
(10.9)

\[
FI = \nabla(Y_{O_2}) \cdot \nabla(Y_{CH_4})
\]  
(10.10)
where $Y_{F_0}^o$ and $Y_{O_2}^o$ represent pure fuel mass fraction and pure oxygen mass fraction, respectively. In the premixed flame region FI is $>0$ and in non-premixed region FI is $<0$. As observed in Fig. 10.17, the peak value of fuel mixture fraction ($Z$) is 20-30 times higher in magnitude for jet-in-cross flow fuel injection case compared to perfectly premixed case. As expected, lower $Z$ value corresponds to higher level of premixedness and which is obviously higher for perfectly premixed case compared to other case where the higher $Z$ is observed around cross-flow fuel injection zone. Interestingly for perfectly premixed case, the higher $Z$ value is observed in the flame tip location and that propagates upstream along with the flame front. Figure 10.18 shows local FI contours for these two different fuel injection systems along the vicinity of flame front during flashback. As noted, FI is always $>0$ for perfectly premixed cases while in jet-in-cross flow case FI is $>0$ inside the flame front (premixed burning region) and $<0$ outside the flame front (non-premixed region). These observations also support the fact why perfectly premixed case exhibits more flashback prone behavior.

A close-up look at the vorticity budget terms (Eq. 10.1) supports the above phenomena, which contributes to the generation of negative azimuthal vorticity, in turn produces the induced negative velocity. Fig. 10.19 shows the time difference distribution of budget terms between $t=9.0s$ and $t=15.0s$ for perfectly premixed case. The upstream propagation of the flame front is due to increase of the induced negative velocity (Eq. 10.4). The analysis clearly reveals that the combined effects of vortex stretching and baroclinic production give rise to the negative azimuthal vorticity particularly along the flame front, while the vortex expansion and diffusion terms stabilize each other influences. Since negative azimuthal vorticity induces negative axial velocity, vortex stretching and baroclinic production are primarily responsible for upstream flame propagation and leading to flashback. Moreover, Fig. 10.16 also supports this fact that the flame tip encounters much higher negative induced velocity in between $t=9.0s$ and $t=12.2s$ due to
Figure 10.19: Individual terms of vorticity transport equation (Eq. 10.1) for S=0.82 with perfectly premixed inlet during flashback: isotherms in black lines
Figure 10.20: Stream lines colored with Damköhler (Da) number contours for $S=0.82$: (a) perfectly premixed inlet, (b) jet-in-cross-flow fuel injection: isotherms in black lines
combined effect of vortex-stretching and baroclinic production and that increases consistently. However, jet-in-cross flow case also exhibits similar behavior but the upstream flame propagation is only delayed compared to perfectly premixed case. Further, the distribution of Damköhler number \( Da \) (Fig. 10.20) also supports the flame propagation during flashback for perfectly premixed case. The plots (Fig. 10.20) show stream lines colored with \( Da \) which is representation of turbulence-chemistry interaction during flashback. Figure 10.20 exhibits the region with low \( Da \) (stronger quenching zone) in the burnt region (inside the flame front) as well as along the reaction zone of flame front. Also, this low \( Da \) region increases as the flame tip moves upstream, including radial broadening of reaction zone. Higher \( Da \) regions are observed outside the flame front, which reveals lower quenching due to fast chemical reaction (low chemical time scale). Usually, the stronger quenching (larger region of small \( Da \)) gives rise to the production of sufficient negative vorticity, which favors upstream flame propagation during flashback. Hence, this observation confirms that higher chemical reaction leads to CIVB and promotes upstream flame propagation.

### 10.2.2.3 Effects of Geometry (Step)

Here the flow configuration has fixed swirl strength of \( S=0.82 \) and assumes everything is premixed at the upstream inlet (Fig. 9.3) based on \( \phi=0.7 \). Once set-up has the ‘step’ in upstream mixing tube, other one does not have any ‘step’ in the mixing tube.

Figure 10.21 shows the time-averaged temperature profiles for perfectly premixed inlet with ‘step’ and ‘without step’ at particular swirl strength. The observation reveals that both the systems exhibit flashback and the flame moves upstream of the dump plane to premixing section and stabilizes there. Notably, the setup with ‘step’ rather shows more susceptible to flashback prone. The interesting phenomenon observed here is that the temperature in the product region (behind the center-body) is less for the case (‘without step’) due to higher flow acceleration in the upstream delivery tube in presence of lower annulus (without the step in the geometry), while the other setup (‘step’) produces much higher temperature regions due to existence of low velocity in B/L in
presence of step. Although, both the system shows flashback prone, the burner ‘without step’ may be useful for lowering NOx production due to lower temperature generation in the burnt regions.

Figure 10.21: Time averaged temperature contours (K scale) at S=0.82 for perfectly premixed inlet: (a) with step, (b) without-step

Figure 10.22 shows the time series temperature plots for the case ‘without step’. The key thing is to be noted here is that the upstream flame propagation for this case (‘without step’) is delayed compared to other case (‘step’, Fig. 10.15). As noticed for this case (‘without step’), the flame front has only reached upto X/2D∼0.5 into the mixing tube at t=9.0s due to recirculation bubble
movement, while in the other case (‘step’) the flame front has moved up to X/2D~2.0 at same time instant (Fig. 10.15). These observations confirm the fact that the step has an impact on upstream flame movement. Here, the flash back is initiated due to Combustion Induced Vortex Breakdown (CIVB) and then accompanied with the favorable condition, due, in part, higher chemical reaction in presence of hydrogen. Since both the cases has perfectly premixed mixture, the flame front always encounters rich fuel region during its upstream movement, while the presence of ‘step’ (Fig. 10.15) provide some additional favorable condition by generating low velocity region in the B/L along the bluff-body wall. This CIVB is often accompanied by a large recirculation zone with high reverse flow velocities in combustions systems. Hence, the reverse velocities bring the heat and reactive species back to the flame tip and maintain the balance between flame tip and flow field at the dump plane. However, the position and motion of this recirculation bubble is very sensitive to the flow field and largely depends on the balance maintained between the induced velocity and irrotational axial velocity. As the region of recirculation zone gives rise to the production of azimuthal vorticity (positive or negative) component in this region, the induced velocity (positive or negative) is generated due to such azimuthal vorticity. Hence, slight changes in the flow field can alter this balance and result in the upstream movement of the recirculation bubble. Once the unsteady motion of recirculation bubble pushes the flame front in the mixing tube, thereafter it encounters higher negative induced velocity due to production of negative azimuthal vorticity. As observed earlier for the case with ‘step’ in Fig. 10.16, formation of such bubble due to vortex breakdown including the movement of the stagnation point (as bubble moves) into the upstream mixing tube.

Considering the perfectly premixed inlet case ‘without step’, the upstream flame movement is also initiated due to upstream propagation of recirculation bubble. Evidently for this case (‘without step’) also, upstream flame propagation occurs due to CIVB, which is less intensive
Figure 10.22: Instantaneous flame propagation for S=0.82: perfectly premixed inlet & without-step (Temperature in K scale)

Figure 10.23: Individual terms of vorticity transport equation (Eq. 10.1) for S=0.82; perfectly premixed inlet & without-step: during flashback
Figure 10.24: Stream lines colored with Damköhler (Da) number contours for $S=0.82$; perfectly premixed inlet & without step: isotherms (black lines)
Figure 10.25: Time averaged temperature contours (K scale) for perfectly premixed inlet without step: (a) S=0.38, (b) S=0.82

compared to other case (‘step’) as shown in Fig. 10.22. The reason behind this is that the negative induced velocity becomes much higher than the low axial velocity in B/L, formed due to ‘step’; and thereby aggressively favors the upstream flame movement for the setup with ‘step’ (Fig. 10.15) while in the other case (‘without step’) incoming flow accelerates more in upstream delivery tube due to lower annular area and does not allow the flame propagation velocity to be dominant over incoming axial velocity for a while resulting delayed occurrence of flashback in this case (Fig. 10.22). Hence, the initiation of flashback occurs at earlier time instants (t=9.0s, Fig. 10.15) for the case with ‘step’, while it is delayed in the other case (‘without step’, Fig. 10.22). Both these cases have perfectly premixed inlet condition that actually favors CIVB due to higher chemical reaction in presence of highly combustible H₂ mixture. Detailed observation of vorticity budget terms (Eq. 10.1) supports the above phenomena, which contributes to the generation of negative azimuthal vorticity, in turn produces the induced negative velocity. Fig. 10.23 shows the time difference distribution of budget terms between t=10.2s and t=15.2s for the
Figure 10.26: Instantaneous flame propagation for $S=0.38$: perfectly premixed inlet & without-step (Temperature in K scale)
case ‘without step’. The upstream propagation of the flame front is due to increase of the induced negative velocity (Eq. 10.4). The analysis clearly exhibits that the combined effects of vortex stretching and baroclinic production give rise to the negative azimuthal vorticity particularly along the flame front, while the vortex expansion and diffusion terms stabilize each other influences. Since negative azimuthal vorticity induces negative axial velocity, vortex stretching and baroclinic production are primarily responsible for upstream flame propagation and leading to flashback. Moreover, Fig. 10.22 also supports this fact that the flame tip encounters much higher negative induced velocity in between t=9.0s and t=12.2s due to combined effect of vortex-stretching and baroclinic production and that increases consistently. Whereas the setup with ‘step’ also exhibits similar behavior where the combined effect of baroclinic production and stretching promotes upstream flame propagation (shown in Fig. 10.19), but the only difference is that the upstream flame propagation takes place early (Fig. 10.15) as noted previously. Further, the distribution of Damköhler number ($Da$) (Fig. 10.24) also supports the flame propagation during flashback for the case ‘without step’. The plots (Fig. 10.24) clearly show the region with low $Da$ increases including radial broadening as the flame front moves upstream. The region of small $Da$ corresponds to the quenching of the reaction, while the regions with large $Da$ correspond to the fast chemical reaction time that prevents local quenching. All the plots in Fig. 10.24 show regions with low $Da$ in the burnt region (inside the flame front) as well as along the reaction zone of flame front. In the stable flame condition upto t=9.0s (Fig. 10.24) the smaller quenching zone (small $Da$ region) does not produce sufficient negative azimuthal vorticity to favor upstream propagation of the flame front. However, when the flame front is pushed further upstream due to recirculation bubble, the stronger quenching (larger region of small $Da$) gives rise to the production of sufficient negative vorticity, which favors upstream flame propagation during flashback as seen in Fig. 10.24 (t=12.2s-17.6s). Hence, the observed phenomena confirm that change in geometry
definitely has some impact on CIVB, but not good enough to avoid occurrence of flashback with hydrogen enriched mixture.

10.2.2.4 Effects Geometry (Step) and Swirl

Here the flow configurations have different swirl strengths: $S=0.38$ and $S=0.82$ and assumes everything is premixed at the upstream inlet (Fig. 9.3) based on $\phi=0.7$.

Figure 10.25 shows time averaged temperature contours for different swirl strength with perfectly premixed inlet. As observed the step with higher swirl ($S=0.82$) exhibits flashback as discussed in the previous subsection. Moreover, the effect of different swirl with jet-in-cross flow fuel injection is also discussed in the subsection ‘effect of swirl’ where the key observation was that the flame does not flashback at lower swirl strength ($S=0.38$). Here in the present scenario, the setup is perfectly premixed (fuel rich condition compared to jet-in-cross flow fuel injection) and operated under lower swirl strength ($S=0.38$). The result reveals the same fact that the flame does not flashback at lower swirl strength ($S=0.38$) even with perfectly premixed mixture. Hence, it can be confirmed that systems with higher swirl become more susceptible to flashback prone, especially with hydrogen enriched mixtures. Fig. 10.26 supports the impact of swirl on instantaneous flame propagation compared to Fig. 10.22. As observed in Fig. 10.26, the flame front is never pushed into the mixing tube due to CIVB (as discussed earlier subsections). Only the flame tip shows a little upstream movement (Fig. 10.26), but thereafter it does not encounter any favorable conditions to promote further upstream movement; such as turbulence, low velocity B/L. Lowering swirl intensity implicitly means lowering the level of turbulence, and thus altering the chemical reaction to reduce the effects of CIVB. Obviously, in the case with low swirl, azimuthal vorticity production is lower (as discussed under the subsection (a) ) and thus does not favors any upstream flame movement. Even though highly combustible hydrogen enriched mixture does not exhibit flashback.

In summary, the above observations confirm the parametric effects on CIVB and flashback
behavior for hydrogen enriched prefixed flame. The flame contributes to vortex breakdown, and results a low or negative flow region ahead of it (recirculation bubble formation with a stagnation point). As the flame tip moves forward, causing the vortex location breakdown region to advance further upstream. This process continues as the flame proceeds further and further upstream. In majority, swirl has a huge impact on CIVB as well as premixedness upto certain extent, especially for hydrogen enriched premixed flames.

10.3 Conclusions

LES with a TF model is used to investigate hydrogen enriched premixed flames in a laboratory based model combustor. The effect of swirl, geometry and premixedness is investigated for hydrogen enriched premixed flame, especially in the context flame flashback. Upstream flame propagation driven by Combustion Induced Vortex Breakdown (CIVB) is known to be a severe problem for premixed swirl burners, and has been investigated in great details. A CIVB driven flame flashback for swirled burner is investigated and reported here on the basis of the of the source terms of the vorticity transport equations. A 2-step chemical scheme for methane combustion and 1-step for hydrogen combustion are invoked to represent the flame chemistry for methane-hydrogen-air combustion. The equivalence ratio for the flame is 0.7 and the Reynolds number is Re=13339 with 30%H₂ mixture. This study leads to the following conclusions:

(a) LES-TF model is able to properly capture hydrogen enriched combustion behavior.
(b) The reacting velocity profiles are well predicted.
(c) Higher swirl broadens the size of recirculation zone for a fixed H₂ enriched mixture.
(d) Increase in swirl strength always leads to flame flashback due to higher turbulence, thus enhances chemical reaction.
(e) Premixedness upto certain extent also affects the flashback behavior. At a particular swirl strength (S=0.82), perfectly premixed mixture tends to behave more flashback prone.
(f) Geometry change has a little impact on flashback behavior at S=0.82.
(g) CIVB driven flame propagation is driving mechanism even for a center-body stabilized swirled burner, and the flame changes the vorticity of the flow field due to its gas-expansion and baroclinic production.

(h) CIVB driven flashback is governed by the interaction of turbulence and the chemistry due to its influence on the vorticity. That’s why higher swirl always show flashback.

(i) The vortex stretching and baroclinic production contribute to the net vorticity generation leading to the occurrence of CIVB driven flashback which produces considerable levels of negative axial velocity that favors upstream flame propagation.

(j) If the flame does not produce enough baroclinic torque, then the combined effects of gas-expansion and diffusion can stabilize the vortex flow and prevent flashback. At lower swirl strength the baroclinic torque is balanced by vortex stretching and does not produce any favorable condition for flashback.

(k) The present study reveals that swirl and premixedness has affect on CIVB driven flashback mechanism in a center-body stabilized swirled burner.

This study demonstrates that the Thickened-Flame based LES approach with simplified chemistry for reacting flows is a promising tool to investigate reacting flows in complex geometries.
Chapter 11 Concluding Remarks and Future Directions

11.1 Summary of the Present Research

Thickened Flame (TF) approach on LES framework has been implemented to study complex turbulent reacting flows. A number of variants of thickened flame model have also been implemented to examine the model performances. Moreover, a modified version of TF model is derived to improve the existing model parameters and investigated. The numerical method uses the primitive variables, which are collocated in both space and time.

Motivated by the limitations of existing combustion models to predict premixed and partially premixed flames, such as those occurring in gas turbine combustors, the models involving thickened flame approaches have been implemented. These methods have capability of handling the chemical kinetics without making any ad-hoc assumptions.

In Thickened Flame (TF) model, the flame front is artificially thickened to resolve it on computational grid points where reaction rates from kinetic models are specified using reduced mechanisms. The influence of turbulence is represented by a parameterized efficiency function. The major advantage associated with this TF model is the ability to capture the complex swirl stabilized flame behavior which is often found in a gas turbine combustor. Since this type of geometry with the premixing section does not guarantee a perfectly premixed gas at the dump plane, the fully premixed assumption in the numerical model is not valid any more. The present TF model is capable of taking care of this type of partially premixed gas since it directly solves for the individual species transport equations and the reaction rates are specified using Arrhenius expressions.

In order to validate the Large Eddy Simulation (LES) code, a number of validation benchmarks are undertaken for general configurations relevant to the geometry of interest. Firstly, turbulent
flow over a backward facing step, isothermal swirling flow in a confined geometry has been studied and predictions are compared with experiments. The aim is to examine the capability of LES for the prediction of turbulent flows with and without swirl. LES successfully captures the vortex breakdown, and the anisotropic turbulence structure for the considered swirl number (S=0.6) with appropriate inflow, outflow boundary conditions, and the needed grid resolution. Good agreement with data is obtained that validates the LES model used.

Further, the piloted premixed stoichiometric methane-air flame for Reynolds number Re = 24,000 on Bunsen burner type geometry (Chen et al., 1996) has been simulated and the original TF model and its variants including the Power-law flame wrinkling model, and the dynamically modified version of these models in conjunction with two different chemistry models have been implemented and compared with experimental data as well as with other published model predictions (PDF and G-eqn). The results indicate that the various variants of TF model produce close agreement with each other using 2-step chemistry model. However, they do exhibit some differences while using 1-step chemistry. Moreover, the 2-step chemistry model appears to perform better over 1-step chemistry model. The original TF model predictions with 2-step chemistry have been found to be in satisfactory agreement with the experimental data and with the more detailed PDF simulations. The mean reaction progress variable and the mean axial velocity are well predicted in the near-field while showing some discrepancies at the downstream locations. The turbulent kinetic energy is under-predicted in the vicinity of the centerline at axial locations X/D=2.5, but matches well at the locations X/D=4.5-8.5. The major species mass fraction predictions are also in good agreement with the exception of CO that is under-predicted by the TF model and over-predicted by the PDF model. In general, the TF model and the previously published PDF model predictions are in reasonable agreement with each other and experiments, whereas the G-equation model predictions show poor performance.
In addition, the predictive capability of modified Thickened Flame (TF) model is also examined on the same stoichiometric Bunsen flame for the Reynolds number Re = 24,000 and 52,000. Detailed results using the modified TF model with thickening factor of 10 (F=10) and pilot temperature of 2005 K have been obtained with a 2-step chemistry model. These results have also been compared with the measurements as well as with other RANS based simulation results using a PDF model and a G-equation model. Moreover, the modified TF model predictions are compared with the original TF predictions, and a number of parameters like thickening factor (F) and pilot boundary conditions are also investigated. It has been found that both the TF models produce very comparable predictions except some modest improvements in mean axial velocity predictions for both flames (F1 & F3) with the modified TF model. The effect of thickening factor is primarily observed in turbulent kinetic energy predictions, while pilot boundary conditions only affect the mean temperature profile. In general, the modified TF model predictions with 2-step chemistry have been found to be in good agreement with the data and show improvement in results in the case of high Reynolds number. The mean axial velocity is well predicted for both the flames, i.e. flame F3 (Re=24000) and flame F1 (Re=52000), but shows higher spreading rate at the downstream locations, especially for low Reynolds number case. In the flame region for flame F3 (Re=24000), the mean reaction progress variable appears to be under predicted along the inner flame brush region, but matches well with the data in the case of flame F1 (Re=52000). The turbulent kinetic energy is under-predicted in the vicinity of the centerline in the near field of injection for both the flames, but is generally well captured at the downstream locations. The major species mass fraction predictions are also in good agreement for both the flames, excluding the CO prediction that is consistently under-predicted. Comparing other model predictions, the RANS based PDF model simulations generally are in reasonable agreement with the data and the TF model except for an over-prediction of the kinetic energy at the lower Re and a significant...
over-estimation of the CO levels. The other RANS based approach, G-eqn. model predictions, are usually not in good agreement with the data; they show a radial-shift of the flame brush region, an over-estimation of the progress variable and CO at the lower Reynolds number. Moreover, the LES coupled G-eqn predictions also do not show good agreement with the data, especially for the lower Re.

Secondly, the validated LES based TF model is used to investigate unconfined swirling flows in a laboratory based model combustor. Both reacting and non-reacting flow conditions for different Reynolds numbers are studied. A 2-step chemical scheme is invoked to represent the flame chemistry for methane-air combustion. The equivalence ratio for the flame is 0.7 and the geometric swirl number for the configuration is 0.82. Isothermal flow predictions are in good agreement with the measurements and indicate that the boundary conditions and grid are properly chosen. Reynolds number is seen to have an impact on the flow field particularly for the non-reacting cases. At a high Re, all the recirculation zones, such as WRZ, CRZ and CTRZ (caused due to vortex breakdown), are clearly observed. At lower Re, the CTRZ is a weaker structure that exhibits a low-frequency unsteady flapping. For the reacting flows, the mean axial velocity profiles are in found to be in good agreement with measurements, and slightly over-predicted close to the dump plane locations. This over-prediction is reflected by a more compact and attached flame in the predictions compared to the experimental observations which show a slightly lifted flame. Moreover, the predicted RMS fluctuations exhibit double peak in the burnt and un-burnt regions and on either side of the peak heat release. In addition, the measured and predicted heat release distributions are in qualitative agreement with each other and exhibit the highest values along the inner edge of the shear layer, while the flame region seen to be more compact with increasing Reynolds number.

Finally, the LES with TF model is used to investigate flashback behavior in hydrogen-enriched
premixed swirled combustor. The results show that higher combustibility of hydrogen causes flame flashback due to complex interaction of chemical reaction in swirled burner, resulting in faster flame propagation. Moreover, the observations reveal that Combustion Induced Vortex Breakdown (CIVB) drives flame flashback in this center-body stabilized swirled burner. It exhibits the upstream propagation of recirculation bubble, which pushes the flame front in the upstream mixing tube and thereafter the flame front moves further upstream due to favorable condition. In particular, combined effect of baroclinic production and vortex stretching accelerates the upstream flame propagation in hydrogen-enriched mixture, while only CH4 shows stable behavior. Moreover, the effect of swirl strength, premixedness and geometry has also been studied on flashback behavior. The analysis reveals that higher swirl strength and increase in level of premixedness make the system more flashback prone due to higher combustibility of hydrogen. Furthermore, flame flashback is always observed at higher swirl strength irrespective of level of premixededness and burner geometry, whereas the premixed systems exhibit stable behavior while operating under lower swirl strength.

In comparing the computational resources, the TF model is always been less computationally expensive compared to PDF model where the use of a look-up table takes substantial computational input/output (I/O) requirements. However, TF model simulations at this stage are restricted to very few number of chemical kinetics (1 or 2-step chemistry) while producing reasonably good agreement of the data. The present research demonstrates that the Thickened-Flame based LES approach with simplified chemistry for reacting flows is a promising tool to investigate reacting flows in complex geometries.

11.2 Future Research Directions

Based on the research conducted so far a part of this dissertation effort, it is possible to identify some challenging and at the same time useful topics for future research.

(a) The thickened flame approach presented in this study provides useful information to
the reacting flow models; it is by no means a complete combustion model, but rather a first step towards a more general approach. In its present form, this approach can account for most of the phenomenological details, however needs improvements. Since this model uses lots of model parameters, which need to be further investigated to improve the performance of the models. The existing parameterization of the model parameters is based on the DNS data sets of 2D classical flame-vortex interaction results (Colin et al., 2000). Using a broader range of data sets that incorporate swirl, separation and other real effects for defining the TF model parameters would be appropriate, but such data sets that provide the needed turbulent-chemistry correlations are not available. Hence further research can be continued in that direction to come up with better model parameters for a broader class of problems.

(b) TF model modifies the diffusion term through artificial thickening which makes the species transport equation more diffusive in nature. This fact can prohibit capturing fundamental combustion phenomena such as ignition, quenching, flame properties due to non-incorporation of detailed chemistry in TF model and that remains a challenging task and can be further addressed.

(c) Flame-holding, thermo-acoustic instabilities in hydrogen rich or pure hydrogen fuel still remains a challenging issue in swirl stabilized burner. Further research can be continued to understand the effect of hydrogen on these key performance metrics.
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Appendix A  Jacobian Matrices

A.1  Conserved Variable Jacobian

The conserved variable Jacobian, $\partial_{\tilde{U}} \tilde{Q}$ used in the unsteady term is expressed as:

$$
\partial_{\tilde{U}} \tilde{Q} = \begin{bmatrix}
\frac{W_1}{RT} & 0 & \ldots & 0 & 0 & 0 & 0 & -\frac{\rho_t}{T} \\
0 & \frac{W_2}{RT} & \ldots & 0 & 0 & 0 & 0 & -\frac{\rho_t}{T} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & \ldots & \frac{W_N}{RT} & 0 & 0 & 0 & -\frac{\rho_N}{T} \\
\frac{u}{RT} & \frac{u}{RT} & \ldots & \frac{u}{RT} & \rho & 0 & 0 & -\frac{\rho w}{T} \\
\frac{v}{RT} & \frac{v}{RT} & \ldots & \frac{v}{RT} & \rho & 0 & 0 & -\frac{\rho w}{T} \\
\frac{w}{RT} & \frac{w}{RT} & \ldots & \frac{w}{RT} & 0 & 0 & \rho & -\frac{\rho w}{T} \\
\Lambda_1 & \Lambda_2 & \ldots & \Lambda_N & \rho u & \rho v & \rho w & \partial_T E_t \\
\end{bmatrix}
$$

(A.1)

where the symbols are defined as

$$
\Lambda_i = \frac{1}{\gamma - 1} + \frac{W_i}{RT} \frac{1}{2} \left( u^2 + v^2 + w^2 \right) \\
E_i = \rho \left[ e + \frac{1}{2} \left( u^2 + v^2 + w^2 \right) \right] \\
\partial_T E_t = \frac{\rho T}{\gamma - 1} - \frac{\rho}{T} \left[ e + \frac{1}{2} \left( u^2 + v^2 + w^2 \right) \right]
$$

(A.2)

A.2  Inviscid Flux Jacobian

The generic expression for the convective part of the inviscid flux Jacobians, $\partial_{\tilde{U}} \tilde{E}, \partial_{\tilde{U}} \tilde{F}$ and
\( \partial_t \tilde{G} \) is expressed for a generalized N-species reacting system as:

\[
\begin{bmatrix}
\frac{U W_1}{RT} & 0 & \ldots & 0 \\
0 & \frac{U W_2}{RT} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \frac{U W_N}{RT}
\end{bmatrix}
\begin{bmatrix}
u W_1^{\kappa_x} \\
\nu W_2^{\kappa_x} \\
\vdots \\
\nu W_N^{\kappa_x}
\end{bmatrix}
\]

\[
\partial_t \tilde{P} = \begin{bmatrix}
\rho_1^{\kappa_x} & \rho_1^{\kappa_y} & \rho_1^{\kappa_z} & -\frac{\rho_1 U}{T} \\
\rho_2^{\kappa_x} & \rho_2^{\kappa_y} & \rho_2^{\kappa_z} & -\frac{\rho_2 U}{T} \\
\vdots & \vdots & \vdots & \vdots \\
\rho_{N-1}^{\kappa_x} & \rho_{N-1}^{\kappa_y} & \rho_{N-1}^{\kappa_z} & -\frac{\rho_{N-1} U}{T} \\
\rho (U + \nu \kappa_x) & \rho (U + \nu \kappa_y) & \rho (U + \nu \kappa_z) & -\frac{\rho U}{T} \\
\rho (U + \nu \kappa_x) & \rho (U + \nu \kappa_y) & \rho (U + \nu \kappa_z) & -\frac{\rho U}{T} \\
\vdots & \vdots & \vdots & \vdots \\
\rho (U + \nu \kappa_x) & \rho (U + \nu \kappa_y) & \rho (U + \nu \kappa_z) & -\frac{\rho U}{T}
\end{bmatrix}
\]

where \( U = \nu \kappa_x + \nu \kappa_y + \nu \kappa_z \) is the Contavariant component of velocity, the generic metric terms are \( \kappa = \xi \) for \( \tilde{P} = \tilde{E} \), \( \kappa = \eta \) for \( \tilde{P} = \tilde{F} \), and \( \kappa = \zeta \) for \( \tilde{P} = \tilde{G} \).

### A.3 Viscous Flux Jacobian

The generic expression for the viscous flux Jacobians, \( \partial_{\tilde{U}} \tilde{P}_v \), is written for a generalized
N-species reacting system as

\[
\begin{bmatrix}
\lambda D_{i m} \beta_1 (1 - Y_1) & \lambda D_{i m} \beta_2 Y_1 & \ldots & \lambda D_{i m} \beta_N Y_1 \\
\lambda D_{i m} \beta_1 Y_2 & \lambda D_{i m} \beta_2 (1 - Y_2) & \ldots & \lambda D_{i m} \beta_N Y_2 \\
0 & 0 & \ldots & 0 \\
0 & 0 & \ldots & 0 \\
\lambda \beta_1 (h_1 - h_m) & \lambda \beta_2 (h_2 - h_m) & \ldots & \lambda \beta_N (h_N - h_m)
\end{bmatrix}
\]

\[
\partial U \tilde{P}_v = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\begin{bmatrix}
\mu_e \left( \lambda + \frac{\kappa_2^2}{3} \right) & \mu_e \frac{\kappa_2 \kappa_\eta}{3} & \mu_e \frac{\kappa_2 \kappa_\eta}{3} & 0 \\
\mu_e \frac{\kappa_2 \kappa_\eta}{3} & \mu_e \left( \lambda + \frac{\kappa_2^2}{3} \right) & \mu_e \frac{\kappa_2 \kappa_\eta}{3} & 0 \\
\mu_e \frac{\kappa_2 \kappa_\eta}{3} & \mu_e \frac{\kappa_2 \kappa_\eta}{3} & \mu_e \left( \lambda + \frac{\kappa_2^2}{3} \right) & 0 \\
\Pi_u & \Pi_v & \Pi_w & k_e \Lambda C_{pm}
\end{bmatrix}
\]

where the generic terms are \( \kappa = \zeta \) for \( \tilde{P}_v = \tilde{E}_v, \kappa = \eta \) for \( \tilde{P}_v = \tilde{F}_v \), and \( \kappa = \zeta \) for \( \tilde{P}_v = \tilde{G}_v \), and

\[
\lambda = \kappa_2^2 + \frac{\kappa_2^2}{3} + \kappa_2^2
\]

\[
\beta_i = \frac{\Pi_u}{u} \left[ u \left( \lambda + \frac{\kappa_2^2}{3} \right) + v \frac{\kappa_2 \kappa_\eta}{3} + w \frac{\kappa_2 \kappa_\eta}{3} \right]
\]

\[
\Pi_u = \mu_e \left[ u \left( \lambda + \frac{\kappa_2^2}{3} \right) + v \frac{\kappa_2 \kappa_\eta}{3} + w \frac{\kappa_2 \kappa_\eta}{3} \right]
\]

\[
\Pi_v = \mu_e \left[ u \frac{\kappa_2 \kappa_\eta}{3} + v \left( \lambda + \frac{\kappa_2^2}{3} \right) + w \frac{\kappa_2 \kappa_\eta}{3} \right]
\]

\[
\Pi_w = \mu_e \left[ u \frac{\kappa_2 \kappa_\eta}{3} + v \frac{\kappa_2 \kappa_\eta}{3} + w \left( \lambda + \frac{\kappa_2^2}{3} \right) \right]
\]

A.4 Chemical source Jacobian

The generic expression for the chemical source term Jacobian (with gravitational terms) \( \partial U \tilde{H} \)
is written for the generalized N-species reacting system as

\[
\begin{bmatrix}
\partial_{p_1}S_1 & \partial_{p_2}S_1 & \cdots & \partial_{p_N}S_1 & 0 & 0 & 0 & \partial_T S_1 \\
\partial_{p_1}S_2 & \partial_{p_2}S_2 & \cdots & \partial_{p_N}S_2 & 0 & 0 & 0 & \partial_T S_2 \\
0 & 0 & \cdots & 0 & \cdots & \cdots & \cdots & \cdots \\
\partial_{p_1}S_N & \partial_{p_2}S_N & \cdots & \partial_{p_N}S_N & 0 & 0 & 0 & \partial_T S_N \\
W_{19x} & W_{29x} & \cdots & W_{N9x} & 0 & 0 & 0 & \frac{\rho g_x}{T} \\
\frac{RT}{RT} & \frac{RT}{RT} & \cdots & \frac{RT}{RT} & 0 & 0 & 0 & \frac{\rho g_y}{T} \\
\frac{RT}{RT} & \frac{RT}{RT} & \cdots & \frac{RT}{RT} & 0 & 0 & 0 & \frac{\rho g_z}{T} \\
\Lambda \rho g_x & \Lambda \rho g_y & \Lambda \rho g_z & -\frac{\rho}{T}
\end{bmatrix}
\]

\text{(A.6)}

where \( \gamma = ug_x + vg_y + wg_z \) and \( S_s \), the total change of mass concentration of species \( s \) is written as:

\[
S_s = W_s \sum_{r=1}^{N_R} \left( \gamma_{rs} - \gamma_{rs}' \right) \left( k_{f_r} \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{rj}} - k_{b_r} \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{rj}'} \right)
\]

\text{(A.7)}

the partial derivatives are defined as

\[
\partial_{p_i}S_s = \frac{1}{RT} \partial_{p_i}S_s
\]

\text{(A.8)}

\[
\partial_{p}S_s = \frac{W_s}{\rho} \sum_{r=1}^{N_R} \left( \gamma_{rs}'' - \gamma_{rs}' \right) \left[ \frac{k_{f_r}}{\rho} \left( \sum_{j=1}^{N} \gamma_{rj} \right) \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{rj}} - \frac{k_{b_r}}{\rho} \left( \sum_{j=1}^{N} \gamma_{rj}' \right) \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{rj}'} \right]
\]

\text{(A.9)}

\[
\partial_{T}S_s = W_s \sum_{r=1}^{N_R} \left( \gamma_{rs}'' - \gamma_{rs}' \right) \left( \partial_{T}k_{f_r} \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{rj}} - \partial_{T}k_{b_r} \prod_{j=1}^{N} \left( \frac{\rho Y_j}{W_j} \right)^{\gamma_{rj}'} \right)
\]

\text{(A.10)}

when the \( r \)th reaction is of the form:

\[
k_{f_r} = A_r T^{\alpha_r} \exp \left( -\frac{E_r}{RT} \right)
\]

\[
\partial_{T}k_{f_r} = \frac{k_{f_r}}{T} \left[ \alpha_r + \frac{E_r}{RT} \right]
\]

\text{(A.11)}

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**Appendix B  Glossary**

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARSM(ASM)</td>
<td>Algebraic Reynolds Stress Model</td>
</tr>
<tr>
<td>BFS</td>
<td>Backward-facing step</td>
</tr>
<tr>
<td>BML</td>
<td>Bray-Moss-Libby</td>
</tr>
<tr>
<td>CARS</td>
<td>Coherent Anti-Stokes Raman Scattering</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CMC</td>
<td>Conditional Moment Closure</td>
</tr>
<tr>
<td>CRZ</td>
<td>Corner Recirculation Zone</td>
</tr>
<tr>
<td>DES</td>
<td>Detached Eddy simulation</td>
</tr>
<tr>
<td>DLE</td>
<td>Dry Low Emission</td>
</tr>
<tr>
<td>DLN</td>
<td>Dry Low NO&lt;sub&gt;x&lt;/sub&gt;</td>
</tr>
<tr>
<td>DNM</td>
<td>Detailed Numerical Simulation</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>EBU</td>
<td>Eddy Break Up</td>
</tr>
<tr>
<td>EDC</td>
<td>Eddy-Diddipation Concept</td>
</tr>
<tr>
<td>HSCT</td>
<td>High Speed Civil Transport</td>
</tr>
<tr>
<td>IRZ</td>
<td>Internal Recirculation Zone</td>
</tr>
<tr>
<td>LDA</td>
<td>Laser Doppler Anemometry</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>l.h.s.</td>
<td>left hand side</td>
</tr>
<tr>
<td>LPP</td>
<td>Lean Premixed/Prevaporized</td>
</tr>
<tr>
<td>MPI</td>
<td>Message Passing Interface</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>pdf</td>
<td>probability density function</td>
</tr>
<tr>
<td>PIV</td>
<td>Particle Image velocimetry</td>
</tr>
<tr>
<td>PLIF</td>
<td>Planar Laser Induced Fluorescence</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds Averaged Navier-Stokes</td>
</tr>
<tr>
<td>r.h.s</td>
<td>right hand side</td>
</tr>
<tr>
<td>r.m.s.</td>
<td>Root Mean Square</td>
</tr>
<tr>
<td>RQL</td>
<td>Rich-burn/Quick-quench/Lean-burn</td>
</tr>
<tr>
<td>RSM</td>
<td>Reynolds Stress Model</td>
</tr>
<tr>
<td>SCR</td>
<td>Selective Catalytic Reduction</td>
</tr>
<tr>
<td>SGS</td>
<td>Sub-grid Scale</td>
</tr>
<tr>
<td>SFS</td>
<td>Sub-filter Scale</td>
</tr>
<tr>
<td>STS</td>
<td>Sub-test Scale</td>
</tr>
<tr>
<td>SSM</td>
<td>Scale Similarity Model</td>
</tr>
<tr>
<td>TFC</td>
<td>Turbulent Flame closure</td>
</tr>
<tr>
<td>UHC</td>
<td>Unburnt Hydrocarbons</td>
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### Appendix C Nomenclature

#### Latin symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
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<tbody>
<tr>
<td>$A_L$</td>
<td>Laminar flame front area</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$c$</td>
<td>reaction progress variable</td>
<td>[-]</td>
</tr>
<tr>
<td>$C_{EBU}$</td>
<td>EBU model constant</td>
<td>[-]</td>
</tr>
<tr>
<td>$C_s, C_\mu$</td>
<td>model constant</td>
<td>[-]</td>
</tr>
<tr>
<td>$D$</td>
<td>molecular diffusivity</td>
<td>[m$^2$/s]</td>
</tr>
<tr>
<td>$D_T$</td>
<td>turbulent diffusivity</td>
<td>[m$^2$/s]</td>
</tr>
<tr>
<td>$E(k)$</td>
<td>kinetic energy spectrum</td>
<td>[m$^3$/s$^2$]</td>
</tr>
<tr>
<td>$E$</td>
<td>Efficiency function</td>
<td>[-]</td>
</tr>
<tr>
<td>$f$</td>
<td>frequency</td>
<td>[s$^{-1}$]</td>
</tr>
<tr>
<td>$G$</td>
<td>signed distance to flame surface</td>
<td>[m]</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>turbulent kinetic energy</td>
<td>[m$^2$/s$^3$]</td>
</tr>
<tr>
<td>$l$</td>
<td>integral length scale</td>
<td>[m]</td>
</tr>
<tr>
<td>$l_f$</td>
<td>flame thickness</td>
<td>[m]</td>
</tr>
<tr>
<td>$L_{a^d}, L_{a^c}$</td>
<td>Markstein length</td>
<td>[m]</td>
</tr>
<tr>
<td>$p$</td>
<td>probability function</td>
<td>[-]</td>
</tr>
<tr>
<td>$S$</td>
<td>swirl number</td>
<td>[-]</td>
</tr>
<tr>
<td>$S_{ij}$</td>
<td>strain rate tensor</td>
<td>[s$^{-1}$]</td>
</tr>
<tr>
<td>$s_d$</td>
<td>flame front displacement speed</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$S_L$</td>
<td>laminar flame speed</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$S'_L$</td>
<td>unstretched laminar flame speed</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$S_T$</td>
<td>turbulent flame speed</td>
<td>[m/s]</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------------------</td>
<td>------------</td>
</tr>
<tr>
<td>$T_u$</td>
<td>temperature on the unburnt side of combustion</td>
<td>[K]</td>
</tr>
<tr>
<td>$T_b$</td>
<td>temperature on the burnt side of combustion</td>
<td>[K]</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature</td>
<td>[K]</td>
</tr>
<tr>
<td>$T_{ij}$</td>
<td>SGS stress tensor</td>
<td>[N/m²]</td>
</tr>
<tr>
<td>$t_F$</td>
<td>reaction time scale</td>
<td>[s]</td>
</tr>
<tr>
<td>$t_l$</td>
<td>turbulent integral time scale</td>
<td>[s]</td>
</tr>
<tr>
<td>$t_\eta$</td>
<td>Kolmogorov time scale</td>
<td>[s]</td>
</tr>
<tr>
<td>$t$</td>
<td>time</td>
<td>[s]</td>
</tr>
<tr>
<td>$U,V,W$</td>
<td>mean velocity components</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$U_o$</td>
<td>bulk velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$U_{con}$</td>
<td>mean outflow velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_i$</td>
<td>velocity components</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u',v',w'$</td>
<td>r.m.s. of velocity fluctuation</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$x_i$</td>
<td>coordinate components</td>
<td>[m]</td>
</tr>
<tr>
<td>$Y_i$</td>
<td>mass fraction of species $i$</td>
<td>[-]</td>
</tr>
</tbody>
</table>

**Greek symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>model constant</td>
<td>[-]</td>
</tr>
<tr>
<td>$\alpha_{ij}, \beta_{ij}$</td>
<td>stress tensor</td>
<td>[N/m²]</td>
</tr>
<tr>
<td>$\delta_{ij}$</td>
<td>Kornecker delta</td>
<td>[-]</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>turbulent kinetic energy dissipation rate</td>
<td>[m²/s³]</td>
</tr>
<tr>
<td>$\overline{\phi}$</td>
<td>time averaging, or spatial averaging of $\phi$</td>
<td>[-]</td>
</tr>
<tr>
<td>$\tilde{\phi}$</td>
<td>Favre time averaging or spatial filtering of $\phi$</td>
<td>[-]</td>
</tr>
</tbody>
</table>
\[ \eta \quad \text{Kolmogorov length scale} \quad [\text{m}] \]
\[ \lambda \quad \text{Taylor length scale} \quad [\text{m}] \]
\[ \mu \quad \text{dynamic viscosity} \quad [\text{kg/ ms}] \]
\[ \mu_t \quad \text{turbulent eddy viscosity} \quad [\text{kg/ ms}] \]
\[ \nu \quad \text{kinematic viscosity} \quad [\text{m}^2/\text{s}] \]
\[ \nu_t \quad \text{turbulent kinetic viscosity} \quad [\text{m}^2/\text{s}] \]
\[ \omega_i \quad \text{reaction rate of species} \ i \quad [\text{kg/ m}^3\text{s}] \]
\[ \tau_{ij} \quad \text{stress tensor} \quad [\text{N/ m}^2] \]
\[ \rho \quad \text{density} \quad [\text{kg/ m}^3] \]
\[ \rho_u \quad \text{density on the unburnt side of combustion} \quad [\text{kg/ m}^3] \]
\[ \rho_b \quad \text{density on bunt side of combustion} \quad [\text{kg/ m}^3] \]
\[ \Sigma \quad \text{flame surface density} \quad [\text{m}^{-1}] \]
\[ \Xi \quad \text{flame wrinkling factor} \quad [-] \]
\[ \Omega_{ij} \quad \text{rotation tensor} \quad [\text{s}^{-1}] \]
\[ \Delta \quad \text{LES filter size} \quad [\text{m}] \]

**Nondimensional numbers**

\[ Da = t_F/t_\eta \quad \text{Damköhler number} \]
\[ Ka = t_F/t_\eta \quad \text{Karlovitz number} \]
\[ Le = D_{th}/D \quad \text{Lewis number} \]
\[ Pr = \nu/D_{th} \quad \text{Prandtl number} \]
\[ Re_t = \rho u' l/\mu \quad \text{turbulent Reynolds number} \]
\[ Sc = \nu/D \quad \text{Schmidt number} \]
\[ Sc_t \quad \text{turbulent Schmidt number} \]
\[ \beta = (T_b - T_u)/T_b \quad \text{nondimensional temperature} \]
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Last Name: De
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