MODELING AND SIMULATION OF COMBUSTION DYNAMICS IN
LEAN-PREMIXED SWIRL-STABILIZED GAS-TURBINE ENGINES

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Abstract

This research focuses on the modeling and simulation of combustion dynamics in lean-premixed gas-turbines engines. The primary objectives are: 1) to establish an efficient and accurate numerical framework for the treatment of unsteady flame dynamics; and 2) to investigate the parameters and mechanisms responsible for driving flow oscillations in a lean-premixed gas-turbine combustor.

The energy transfer mechanisms among mean flow motions, periodic motions and background turbulent motions in turbulent reacting flow are first explored using a triple decomposition technique. Then a comprehensive numerical study of the combustion dynamics in a lean-premixed swirl-stabilized combustor is performed. The analysis treats the conservation equations in three dimensions and takes into account finite-rate chemical reactions and variable thermophysical properties. Turbulence closure is achieved using a large-eddy-simulation (LES) technique. The compressible-flow version of the Smagorinsky model is employed to describe subgrid-scale turbulent motions and their effect on large-scale structures. A level-set flamelet library approach is used to simulate premixed turbulent combustion. In this approach, the mean flame location is modeled using a level-set G-equation, where G is defined as a distance function. Thermophysical properties are obtained using a presumed probability density function (PDF) along with a laminar flamelet library. The governing equations and the associated boundary conditions are solved by means of a four-step Runge-Kutta scheme along with the implementation of the message passing interface (MPI) parallel computing architecture. The analysis allows for a detailed investigation into the interaction between turbulent flow motions and oscillatory combustion of a swirl-stabilized injector. Results show good agreement with an analytical solution and experimental data in terms of acoustic properties and flame evolution. A study of flame bifurcation from a stable state to an unstable state indicates that the inlet flow
temperature and equivalence ratio are the two most important variables determining the stability characteristics of the combustor. Under unstable operating conditions, several physical processes responsible for driving combustion instabilities in the chamber have been identified and quantified. These processes include vortex shedding and acoustic interaction, coupling between the flame evolution and local flow oscillations, vortex and flame interaction and coupling between heat release and acoustic motions. The effects of inlet swirl number on the flow development and flame dynamics in the chamber are also carefully studied. In the last part of this thesis, an analytical model is developed using triple decomposition techniques to model the combustion response of turbulent premixed flames to acoustic oscillations.
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Nomenclature

\(A, B, C\)  Jacobian matrices of convective flux

\(C_p, C_v\)  Specific heat, \(J \cdot Kg^{-1} \cdot K^{-1}\)

\(C_R, C_I\)  Empirical constants

\(c\)  Speed of sound, \(m/s\)

\(D\)  Van-Driest damping function

\(E\)  Specific total energy, \(J \cdot Kg^{-1}\)

\(E, F, G\)  Convective flux vector

\(E_v, F_v, G_v\)  Diffusion flux vector

\(f\)  Frequency, \(Hz\)

\(G\)  Level-set variable

\(G_f\)  LES filter function

\(h_{i,j}^0\)  Heat of formation of species \(i\) at reference condition

\(k\)  Turbulent kinetic energy

\(l_F\)  Laminar flame thickness, \(m\)

\(l_\delta\)  Inner-layer flame thickness, \(m\)

\(n\)  Unit vector normal to flame front

\(N\)  Total number of species

\(p\)  Pressure

\(P_r\)  Prandtl number

\(q\)  Rate of heat release per unit volume

\(R\)  Gas constant

\(R_h\)  Radius of center body

\(R_n\)  Radius of inlet duct

\(S\)  Flame speed, or swirl number

\(S_{ij}\)  Strain-rate tensor

\(Sr\)  Strouhal number

\(u_i\)  Velocity, \(m/s\)
Friction velocity, $m/s$

Molecular weight of species $i$

Mass fraction of species $I$

Normalized distance from wall

**Greek Symbols**

$\Delta$  
Filter width

$\delta_{ij}$  
Kronecker delta

$\phi$  
Equivalence ratio

$\varphi$  
Swirler vane angle

$\mu$  
Dynamic viscosity, $kg/ms$

$\tau_{ij}$  
Viscous shear stress, $N/m^2$

$\theta$  
Phase angle

$\rho$  
Density, $kg/m^3$

$\eta$  
Kolmogorov length scale, $m$

$\gamma$  
Ratio of specific heats

$\omega$  
Vorticity, $1/s$

**Subscripts**

$a$  
Acoustic property

$L$  
Laminar property

$rms$  
Root mean square

$T$  
Turbulent property

$\xi, \eta, \zeta$  
Each direction in body fitted coordinate system

**Superscripts**

$sgs$  
Subgrid scale

$-$  
Ensemble averaging

$\sim$  
Favre averaging

$'$  
Fluctuation

$\wedge$  
Complex variable
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Chapter 1

Introduction

1.1 Background and Motivation

Gas-turbine engines have traditionally used diffusion-flame combustors because of their reliable performance and reasonable stability characteristics. Unfortunately, this type of combustor produces unacceptably high levels of thermal NOx. The increasingly strict regulation of pollutant emissions has recently led engine manufacturers to develop low-emissions gas-turbine engines to fulfill the regulatory requirements (Bahr, 1993; Correa, 1993). New concepts of combustion have been introduced into the gas-turbines industry, including Lean Premixed (LPM) Combustion, Rich-Quench-Lean (RQL) Combustion, and Catalytic Combustion (Lefebvre, 1995; Correa, 1998). For these three methods, RQL techniques are hampered by soot formation and incomplete mixing between fuel-rich combustion products and air. Catalytic Combustion suffers from cost, durability and safety. Lean Premixed combustion is probably the most promising combustion technology for practical machines at the present time. Fig. 1-1 shows the LM6000 Dry Low Emission (DLE) Gas Turbine developed by the General Electric Company for land and marine applications. It meets the NOx emissions goal of 25 ppm in site rating conditions by employing the Lean Premixed approach (Mongia, 1998). The term “dry” indicates here that water or steam does not need to be injected to reduce emissions. In LPM combustion, the fuel and air are premixed upstream of the combustor to avoid the formation of stoichiometric regions. The combustion zone is operated with excess air to reduce the flame temperature; consequently, thermal NOx is virtually eliminated. However, unsteady flow oscillations, usually
referred to as combustion instability, have emerged as a common problem due to the near lean-limit operations, hindering the development of LPM combustors. These oscillations in the flowfield may reach sufficient amplitudes to interfere with engine operation. In extreme cases, the ensuing structural vibration and excessive heat transfer to the chamber lead to system failure.

Combustion instabilities may be regarded as unsteady motions in a dynamical system capable of sustaining large oscillations over a broad range of frequencies. Because fluctuations arise from causes internal to the system, they are true instabilities. An external observer perceives the result as the dynamical behavior of a “self-excited” system. The prevalence of instabilities is primarily attributed to two fundamental phenomena (Culick and Yang, 1992, Culick and Yang, 1995):

a) Combustion chambers are almost entirely closed and the internal processes tending to attenuate unsteady motions are weak; and

b) The energy required to drive unsteady motions represents an exceedingly small fraction of the heat released by combustion.

These underlying issues are present in any combustion chamber, but are especially consequential for gas-turbine engines in which energy intensity is extremely high, typically of the order of 100 MW/m³/bar. In typical instances, less than 0.1% of the energy released in chemical reactions is
sufficient to generate pressure fluctuations having peak amplitudes equal to the mean chamber pressure.

The above observations indicate that the possibility of instabilities occurring during the development of new gas-turbine engines must be anticipated and recognized. Stable combustion in the gas turbine combustor may become unstable and instabilities may occur due to small changes in geometry configurations and the manner in which the reactants are introduced. Thus a comprehensive understanding of combustion instability is strongly needed to design modifications. Several mechanisms responsible for driving combustion instabilities, such as hydrodynamic instabilities (Schadow and Gutmark, 1992), equivalence-ratio fluctuations (Lieuwen and Zinn, 1998), and flame surface variations (Fleifil, et al., 1996), have been proposed and studied. Very limited effort, however, has been expended to investigate the detailed flame dynamics, especially at scales sufficient to resolve the energy cascade process in an oscillatory environment. Most LPM systems stabilize the flame with recirculation developed by swirling flows for the purpose of clean and efficient combustion. There are, however, many unresolved issues with respect to swirling flows such as swirl generation, vortex breakdown, axisymmetry breaking, and azimuthal instability (Shtern and Hussain, 1999; Paschereit et al., 2000). Effects of swirling flow on combustion instabilities remain largely unclear, at least in the quantitative sense. The lack of fundamental information about the flame/flow interaction has seriously jeopardized the establishment of a knowledge-based design methodology to cure the instability problem. Hence, the work herein attempts to utilize contemporary numerical and analytical modeling techniques to address various fundamental issues associated with oscillatory flame dynamics in lean-premixed swirl-stabilized combustors.
1.2 Literature Review

1.2.1 General Description of Combustion Instabilities

Oscillations in pressure, velocity, and temperature always exist in a practical combustion system, even in stable operations. Typically, combustion with amplitudes of pressure fluctuations less than about 5% of the mean chamber pressure is usually defined as smooth combustion. Combustion with larger but completely random pressure fluctuations is termed rough combustion, while combustion with periodic pressure oscillations and large amplitudes are referred to as combustion instabilities (Crocco and Cheng, 1956; Weiss, 1966; Sutton and Biblarz, 2000).

Combustion instability may either develop spontaneously within the system or be initiated by any natural or artificial perturbation external to it. The first case is referred to as self-excited instability. Generally, a small perturbation grows out of system noise for some time and eventually displays periodic behavior. Because the oscillations arise from causes internal to the system, they are true instabilities and an external observer perceives the result as the dynamical behavior of a self-excited system. For the latter case, the instabilities are initiated by a finite-amplitude perturbation external to the system, which is otherwise stable to small disturbances (Wicker et al., 1996; Wang, 1997). For any type of instability, the pressure amplitude of oscillations grows with time only if the energy gain from combustion to the oscillation field is greater than the energy lost. Whether or not a pressure perturbation leads to instability depends on the excitation mechanism and the nature of the driving and damping processes.

Depending on the combustion chamber geometry, injector configuration and position, entire system geometry and fuel/air mixture properties in the combustion systems, combustion instability observed in each system displays different characteristics. Even though most of the instabilities observed in different combustion systems are specific to that system, some general
classification can be established to help the understanding of instability mechanisms. One way (Barrère and Williams, 1969; Williams, 1985) to classify combustion instabilities is in terms of components of a combustion system. Three major classes of combustion instabilities are identified: system instabilities, chamber instabilities, and intrinsic instabilities. The characteristics of system instabilities are affected by the interaction between processes occurring within the combustion chamber and those occurring in the other parts of the system, including the fuel supply tanks, fuel lines and the exhaust elements. The second class, chamber instabilities, is usually associated with the occurrence of combustion in the combustor chamber (William, 1985). Chamber instabilities may be induced by acoustic disturbances, shock dynamics and hydrodynamics instabilities within the chamber. Intrinsic instabilities are inherent in the combustion, and may exist irrespective of whether the combustion occurs within a combustion chamber and can be triggered without any external influences (Barrère and Williams, 1969; Candel, 1992; Candel et al., 1996). The intrinsic instabilities may involve chemical-kinetic instabilities, diffusive-thermal instabilities or hydrodynamic instabilities (Clavin, 1985). Among these three classes of instabilities, chamber instabilities are found to occur in many practical combustion systems, including the LPM gas-turbine engines as well as liquid and solid rocket engines, and are of the most interest in the present study.

Combustion instabilities can also be generally categorized by their frequencies and grouped into the following categories: low frequency (chugging), intermediate frequency (buzz) and high frequency (screaming or Screeching) (Sutton and Biblarz, 2000). Chugging instabilities are in the frequency range of 10 to 400 Hz, Screaming (or Screeching) instabilities have frequencies higher than 1000 Hz, Buzz instabilities are in the frequency range between 400 Hz and 1000 Hz. Usually, chugging instability and buzz instabilities are mostly related to the systems, while screaming (or screeching) instabilities are usually linked to chamber instabilities.
1.2.2 Driving Mechanisms of Combustion Instabilities

The heat release from chemical reactions is the main source of energy driving unsteady flow oscillations. Although the energy needed to drive unsteady motions is only an exceedingly small fraction of the heat release from combustion (Culick and Yang, 1992; Culick and Yang, 1995), combustion instabilities cannot be sustained unless a certain dynamic relation between heat release fluctuations and acoustic pressure oscillations is satisfied in the combustion chamber. The dependence of combustion instability on the relationship between heat release and acoustic oscillations was first identified by Lord Rayleigh. In his book *The Theory of Sound*, he explained the excitation of tones in a Rijke tube as follows:

*If heat be periodically communicated to, and abstracted from, a mass of air vibrating (for example) in a cylinder bounded by a piston, the effect produced will depend upon the phase of the vibration at which the transfer of heat takes place. If heat be given to the air at the moment of greatest condensation, or be taken from it at the moment of greatest rarefaction, the vibration is encouraged. On the other hand, if heat be given at the moment of greatest rarefaction, or abstracted at the moment of greatest condensation, the vibration is discouraged.*

(Rayleigh, 1945)

This paragraph gives the so-called Rayleigh criterion for the occurrence of combustion instability. The Rayleigh criterion states that if heat is released when a pressure oscillation is near its maximum, the pressure fluctuations increase in amplitude. On the other hand, if heat release occurs when the pressure oscillation is at a minimum point, pressure fluctuations are attenuated.

The Rayleigh criterion can be obtained mathematically from flow equations using Reynolds decomposition. There are many possible ways to obtain this result (Chu, 1965; Culick, 1988; Candel, 1992; Dowling, 1997). If we consider a combustion process within a cavity of
volume \( V \), enclosed by surface \( S \), combining the linearized equations of mass, momentum and energy, an averaged acoustic energy equation can be derived as follows:

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \overline{\rho u_i'^2} + \frac{1}{2} \overline{\frac{p'}{\rho c^2}} \right) dV + \int (p'u_j' - \overline{u_i' \tau_{ij}'}) dS_j = \int \left( \frac{\gamma - 1}{\rho c^2} p'q' dV - \int \frac{\partial u_i'}{\partial x_j} \tilde{\nu}_j' dV \right)
\]

where \( \tilde{c} = \sqrt{\gamma \overline{RT}} \) is the mean speed of sound. The first term on the left-hand side of Eq. 1.1 is the rate of change in acoustic energy. The second term on the left-hand side accounts for the energy exchange between volume \( V \) and surroundings through surfaces \( S \). The first term on the right-hand side describes the coupling of combustion and pressure acoustic motions. This term tends to increase acoustic energy when heat release and acoustic oscillations are in phase, which, of course, is closely related to the Rayleigh criterion. The last term represents viscous dissipation.

If the combustion system is closed and there is no energy exchange across surfaces \( S \), the second term can be dropped out. When pressure and heat release fluctuations are out of phase, the sum of the two terms on the right-hand side of Eq. 1.1 is negative, meaning that acoustic waves cannot be sustained. If the sum of the two terms on the right-hand side of Eq. 1.1 is greater than zero, pressure oscillations are amplified due to addition of energy from the heat release produced during combustion. In reality, the amplitudes of unstable pressure oscillations cannot grow indefinitely; they are limited by an energy loss process through viscous dissipation and energy exchange across the boundary \( S \). Consequently, the pressure oscillation amplitude will reach a limit when the energy loss becomes equal to the energy gain through nonlinear processes. The prediction of the limit amplitudes must be approached through a nonlinear analysis, although the frequency and mode structure of unstable combustion can be computed through a linear analysis (Crocco, 1951). Note that heat release and pressure oscillations are not
only functions of time, but also space, since the characteristics of heat release change over the finite distance traveled by acoustic waves.

The physical processes responsible for driving combustion instabilities may either modify the heat release fluctuation or pressure oscillations or both. The sources of pressure fluctuations include acoustic motions in the chamber, and hydrodynamics instabilities, etc. Heat release is largely controlled by the local air-to-fuel mixture ratio, mass flow rate, together with instantaneous pressure and temperature. Specifically, for gas-fuel premixed flame, heat-release fluctuations may arise from flame surface variations, equivalence ratio fluctuations, mass flow rate oscillations, and vortex shedding processes due to hydrodynamics instabilities. For liquid fuel, atomization and droplet vaporization are additional sources of heat-release fluctuations. Some specific discussions of sources of pressure and heat release fluctuations are presented in the following subsections.

1.2.2.1 Acoustic Motions in Combustor Chambers

In the dump combustor, perhaps the most problematic type of instability involves coupling of acoustic motions with combustion and can be characterized by an energy feedback loop between the acoustic oscillations and transient combustion processes. One reason for the prevalence of acoustic-coupled instabilities in the gas turbine combustor is the relatively closed acoustic environment within which combustion occurs, and the relatively high amounts of energy available from the combustion to drive the acoustic field (Culick and Yang, 1992). Also, because acoustic waves can propagate both upstream and downstream in subsonic-flow combustion, acoustic disturbances generated anywhere in the chamber may affect the entire reacting flow field, thus providing a path for energy feed-back between the flow processes and the combustion process.
Using Reynolds decomposition, which expresses flow variables as the sum of a mean and a fluctuation part, one can derive a wave equation in the combustion chamber from the conservation equation of mass, momentum and energy (Culick and Yang, 1992; You et al., 2003a) as follows:

\[
\nabla^2 p' - \frac{1}{\bar{c}^2} \frac{\partial^2 p'}{\partial t^2} = h(\vec{U}, \vec{p}, u', p', q', \text{etc.}) \quad (1.2)
\]

subject to boundary condition: \( n \cdot \nabla p' = -f \)

where \( \bar{c} = \sqrt{\gamma R T} \) is the mean sound speed in the chamber and \( h \) is the source term, which includes the effects of unsteady heat addition, mean temperature gradients, and mean flow velocity. If we neglect the source term \( h \) and consider a cylindrical chamber with a closed boundary, by using methods of separation of the variables, the general solution for Eq. 1.2 can be written as:

\[
p' = \sum_{l,m,n} A_{lmn} J_m(k_{rmn}r) \cos(m\theta + \gamma_{lmn}) \cos(k_{zl}z)e^{i\omega_{lmn}t} \quad (1.3)
\]

where \( l, m, \) and \( n \) are integers; \( J_m \) is the Bessel function of the first kind of order \( m \); \( k_{zm}L = l\pi \), where \( L \) is chamber length; \( k_{rmn}R = j'_{mn} \), \( j'_{mn} \) is the \( n \)th extremum of the \( m \)th Bessel function of the first kind; and \( R \) is chamber radius. The allowed angular frequencies are determined from:

\[
\omega_{lmn} = \bar{c}(k_{rmn}^2 + k_{zl}^2)^{1/2} \quad (1.4)
\]

Terms in Eq. 1.3 with \( m = n = 0, \ l \neq 0 \) describe longitudinal modes; those with \( l = m = 0, \ n \neq 0 \) correspond to radial modes; and those with \( l = n = 0, \ m \neq 0 \) represent tangential (azimuthal) modes.
The estimated frequencies of oscillation obtained from the above simple classical acoustics analysis commonly lie within 10-15% or less of the frequencies observed in the experiments for combustion instabilities (Culick, 2001). However, it is precisely the departure from classical acoustics that defines the class of problems we call combustion instabilities. According to Culick (2001), there are three main reasons that the classical view of acoustics is a good first approximation to wave propagation in the combustion chamber. First, the Mach number of the mean flow is usually low so that convective and refractive effects are small. Second, if the exhaust nozzle is choked, the incident waves are efficiently reflected, and the exit plane can be regarded as a rigid surface. Third, in the limit of small amplitude disturbances, the unsteady motion in the compressible flow can be decomposed into three independent modes of propagation, i.e., acoustic wave, vortical wave and entropy wave. Even in the highly turbulent non-uniform flow usually present in a combustion chamber, acoustic waves behave in good first approximation according to their own simple classical laws. (However, the classical linear acoustic analysis cannot decide in which modes the acoustic oscillations will be excited; it also cannot predict the amplitude of the excited frequencies. Those are determined by flow and combustion conditions in the chamber and must be approached through a nonlinear analysis.)

1.2.2 Flame Surface Variations

For a gas-fueled premixed flame, the heat release per unit volume can be expressed as:

\[ \dot{q} = \rho_u S_L A_f \Delta h_f^0 \]

(1.5)

where \( S_L \) is laminar flame speed, \( A_f \) is flame surface area per unit volume, \( \rho_u \) is density of unburnt gas, and \( \Delta h_f^0 \) is heat of reaction per unit mass. Assuming that all properties except the
flame surface area are constant, the ratio of the fluctuations of the heat release rate to the mean heat release rate is proportional to the ratio of the changes in the flame surface area to the average flame surface area.

\[
\frac{\dot{q}'}{\bar{q}} = \frac{A'}{A_f} 
\]  

(1.6)

Usually, an idealized planar configuration does not exist for practical flames. Depending on parametric conditions, a laminar flame may become unstable and wrinkle under intrinsic flame instabilities, resulting in an enhanced flame front area and ultimately leading to self-turbulization of combustion. These intrinsic instabilities, including Darrieus-Landau instability (Landau, 1944) and thermal-diffusive instabilities (Sivashinsky, 1977), have been extensively studied in the past. One complicating feature of the topology of a flame surface in a turbulent flow is that turbulent eddies can wrinkle the flame front. Turbulent eddies can enhance the flame surface areas and consequently increase heat release rate.

Many researchers have investigated the flame surface response to pressure oscillations. Marble and Candel (1978) investigated the flame and acoustic interaction based on thin flame sheet concepts. The non-steady behavior of a flame stabilized by a single-flame holder at the center of a long two-dimensional duct is treated by an integral technique in which relevant equations are integrated across burnt and unburnt gas separately. A perturbation technique is applied to examine the flame response to acoustic distances. Their results indicate that a very active response of the stabilized flame to the incident acoustic wave disturbances occurs at certain frequencies that correspond to well-defined values of \(\omega L / u_0\), where \(L\) is the length of the flame zone and \(u_0\) is the flow velocity upstream of the flame zone. Their model was further extended by Subbaiah (1983) and Yang and Culick (1986). Yang and Culick’s model includes gas compressibility and accommodates the recirculating flow behind the flame holder. Their work
was also the first in which the severe gradients in the properties of the mean flow were accounted for in the analysis of unsteady motions.

Recently, an analytical model describing the dynamic response of a laminar premixed flame stabilized on the rim of a tube to acoustic velocity perturbations was proposed by Fleifil et al. (1996). The model was derived from a linearized flame surface evolution equation. Their results show that the magnitude of heat release and the phase with the dynamic perturbation are strong functions of the flame Strouhal number, which represents the ratio of the dominant frequency times the tube radius to the laminar flame speed, $\omega R/S_L$. It was found that high-frequency oscillations pass through the flame without affecting the heat release significantly, while low frequency perturbations have a strong impact on the heat release fluctuations. This model was later extended by Dowling (1999) using a constant turbulent flame speed to describe the turbulent flame response to flow oscillations.

Flame surface measurements were performed by Reuter et al. (1990) using a phase-locked shadow photography technique. The distortion of flame front, which results from periodic vortex shedding, causes a cyclic variation in the flame surface area and heat release. The role of flame area variations was also investigated experimentally by Venkataraman et al. (1999) in a lean-premixed dump combustor, which indicated that the flame area fluctuations are very nearly in phase with the pressure oscillations.

### 1.2.2.3 Equivalence Ratio Fluctuations

Recently, more and more researchers have recognized the important role of equivalence ratio fluctuations on combustion instability. Equivalence ratio is one of the major sources of heat release fluctuations. Equivalence ratio fluctuations are due to the incomplete mixing of air and
fuel ahead of the flame front or as a result of mass flow fluctuations of air or fuel at the fuel injection location. The former case is due to the limited space and time available for premixing fuel and air in the combustion inlet system. The latter case results from excited pressure oscillations (Seo, 1999). A theoretical investigation of lean premixed combustion oscillations has been given by Lieuwen and Zinn (1998), concentrating on the effects of equivalence ratio fluctuations. Their model extended the basic idea of a simple time lag theory first developed by Crocco and Cheng (1956) through the careful consideration of acoustic boundary conditions and effects of fuel line length. This model was then incorporated into a low NOx gas turbines stability analysis. Their results showed that gas turbines are highly prone to combustion instabilities, especially under lean operating conditions.

One explanation for why lean premixed combustion is more susceptible to instabilities can be given in terms of the relationship between equivalence ratio and chemical reaction time. Small changes in the equivalence ratio near a lean flammability limit can introduce large variations in many characteristics of a flame, such as flame temperature, and chemical time and flame speed. The experimental data obtained by Zukoski (1978), as shown in Fig. 1-2, indicate that the gradient of chemical time, $\partial \tau_{\text{chem}} / \partial \phi$, increases significantly as the flame gets leaner. Since chemical time is inversely proportional to the reaction rate, even a small change in the equivalence ratio can create large fluctuations in the reaction rate at lean conditions compared to the stoichiometric condition. As a result, pressure oscillations grow strongly in amplitude when the fluctuations in the reaction rate are coupled with the acoustics of the combustor system, making a closed loop for the energy transfer mechanism between chemical energy release and the driving of the acoustic pressure field.
The high sensitivity of reaction rate to equivalence ratio oscillations was demonstrated by Lieuwen et al. (1998) in their model of the response of an unsteady well-stirred reactor to equivalence ratio perturbations at lean conditions. Their results indicated that the magnitudes of the reaction rate and heat release oscillations significantly increase as the equivalence ratio decreases under lean conditions. Employing the idea that the effects of equivalence ratio fluctuations are significant in determining the instability characteristics, Richards et al. (1998) were able to suppress pressure oscillations by modulating the fuel flow rate to avoid the unstable operating regime corresponding to specific equivalence ratio conditions.

### 1.2.2.4 Hydrodynamic Instability

The role of fluid dynamic instabilities in changing the heat release rate is also considered in many studies. In a dump combustor, strong shear layers are generally formed at the rearward...
facing steps. Such transitional shear layers are usually characterized by large-scale coherent structures or vortices. The observation and recognition of the importance of the vortex shedding process as a possible mechanism for driving combustion instabilities was first independently reported by Kaskan and Noreen (1955) and by Rogers and Marble (1956), as pointed out by Culick (1988). In particular, the latter work provided an explanation of the mechanism of generating self-excited oscillations through a closed-loop process. Fresh mixture was entrained by vortical structures, and ignition took place after a certain characteristic time. Delayed periodic combustion in shed vortices generated periodic acoustic oscillations. The fluctuating velocity of the acoustic field interacts with shear layers and closes the loop. Since those studies, a great deal of attention has been given to the role of vortex shedding on combustion instabilities (Smith and Zukoski, 1985; Sterling and Zukoski, 1987; Poinsot et al., 1987; Schadow et al., 1989; Schadow and Gutmark, 1992).

The experimental works of Smith and Zukoski (1985) and Sterling and Zukoski (1987) were conducted in a two-dimensional dump combustor and focused mainly on the unsteady combustion associated with vortex motions. Their work showed that acoustic velocity fluctuation causes large vortical structures to shed from the flameholder. Their subsequent development of vortex motions and the associated heat release depends on step height, mean velocity, fuel types and equivalence ratio. Poinsot et al. (1987) investigated vortex-acoustic wave coupled combustion instabilities in a multiple inlet dump combustor. Although the acoustic modes of the combustor can be predicted using linear acoustic analysis, the experimental results showed that combustion instabilities occur only at certain frequencies among the predicted ones, which are determined by the characteristic times of convection and combustion process in the flow. Their spark-schlieren and phase-averaged images of C₂ showed that certain instabilities are vortex driven and the occurrence of vortex shedding is in phase with the acoustic velocity fluctuation.
In a review, Schadow and Gutmark (1992) summarized previous research programs related to the driving mechanism of dump combustor instability, with emphasis placed on vortex shedding as a driving mechanism of combustion instabilities. The evolution, interaction, and breakdown of large-scale structures into small-scale turbulence were described and the interaction between acoustic waves and the shear layer were explored. The shear layer is characterized by several instability frequencies associated with different sizes of vortices. Schadow and Gutmark consistently interpreted distinct frequencies found in their instability experiments in terms of vortex shedding dynamics in the shear layer. When acoustic waves interact with the shear layer, the stabilization of the vortex size depends on the match between acoustic frequency and the shear layer instability frequencies. Their observation indicates that the size of the vortices is smallest when the acoustic frequency equals the initial vortex shedding frequency. It is largest when the acoustic frequency is near the preferred-mode frequency. In non-reacting flow tests, the acoustic emission of the vortices is low. There is no obvious feedback between the flow and the acoustic pressure in the chamber. However, in reacting flow, the large periodic heat release associated with the combustion inside the vortices provides the missing link for the necessary feedback loop. The evolution of coherent flow structures leads to periodic heat release, which, when in phase with the pressure oscillation, can drive the instabilities as stated by the Rayleigh criterion.

1.2.3 Instability Stabilization Methods

The suppression of combustion-inducing pressure oscillations is a major challenge in the design and development of high-performance combustors. Both passive techniques and active techniques have been used. Passive control can be achieved by changing the basic design of the system (geometry, injector type, installation of baffles etc.). In contrast to passive techniques,
active controls utilize external excitation (e.g., loudspeakers, unsteady fuel injection, etc.) to suppress the instability. Both passive and active control techniques have been successfully applied in instability control in many combustion systems.

An example of a passive control approach is baffles, which can provide significant stabilizing effects on pressure oscillations and have been widely used in rocket engines since 1954 (Male and Kerslake, 1954). A typical configuration consists of flat plates extending into a chamber perpendicularly from the injector face. Three mechanisms have been proposed for explaining successful elimination of instability by baffles: (1) modification of acoustic resonance properties (i.e., frequency and waveform); (2) restriction of unsteady motions between baffle blades, and subsequent shielding of the sensitive mechanisms for instabilities; and (3) damping of oscillations by vortex shedding, flow separation, and viscous dissipation (Harrje and Reardon, 1972).

In their effort to control the combustion instability of a DLE Radial-staged combustor, GE used both passive and active control measures. For passive control, they installed damper tubes (which are basically the quarter-wave tubes) in the cold section of the combustor just upstream of the premixers. These damper tubes are used to detune the predominant oscillation frequencies in the combustor by providing finite number of discontinuities at locations where they are installed. Also, so-called Enhanced Lean Blow-Out (ELBO) fuel, which was originally introduced to enhance lean-blow-out performance of the combustor, was injected through equally spaced holes located at the exit of the premixer for active combustion control. (Pandalai and Mongia, 1998)

In both passive and active control techniques, it is critical to expand physical understanding of combustion dynamics for the further development of effective control technology. Since combustion characteristics are closely related to detailed fluid dynamic
processes (Schadow and Gutmark, 1992), the coupling between shear-flow dynamics and heat release mechanisms in a high-swirl environment is one of the major concerns in this study.

1.2.4 Swirling Flows

Many LPM gas-turbine systems utilize swirling flows to stabilize the flame for the purpose of stable, efficient and clean combustion. There are, however, many unresolved issues of swirling flows such as swirl generation, vortex breakdown, axisymmetry breaking and azimuthal instability (Sthern and Hussain, 1999; Paschereit et al., 2000). One of the most important flow characteristics produced by swirl-stabilized injectors is the central toroidal recirculation zone (CTRZ), which serves as a flame stabilization mechanism (Gupta et al., 1984). Flows in this region are generally associated with high shear rates and turbulent intensity resulting from vortex breakdown. Although this kind of flow oscillation promotes the mixing of fuel and air and extends the range of flame stability, it is sometimes not a desirable characteristic because it is prone to drive combustion instabilities. Swirling flows may affect combustion instability in two ways. First, large-scale unsteady motions due to high shear layer and vortex breakdown, as well as precessing vortex core (PVC), induce hydrodynamic instability. The ensuing flow oscillations may couple resonantly with acoustic waves in the combustor, subsequently causing combustion instabilities. Second, swirling flows affect the flame size, flame shape and combustion intensity, and consequently influence heat release distribution in the combustion chamber. The overall influence of the distribution of heat release on combustion instability could be significant.

As the degree of the swirl increases, vortex breakdown takes place. The phenomenon of vortex breakdown, defined as an abrupt change in the character of a vortex core, is manifested with the recirculation zone in the downstream of the center body. The region provides the
mechanisms for flame stabilization, and is characterized by the existence of internal stagnation points and reversed flows. Sarpkaya (1971) first observed three types of vortex breakdowns: double helix, spiral, and axisymmetric (bubble). Later, Faler and Leibovich (1978) revealed seven different types of vortex breakdowns using a liquid dye tracer in their water flow visualizations. Among them, bubble and spiral modes of breakdown were commonly observed in swirl-stabilized gas-turbine combustors. The bubble mode usually prevailed at high swirl numbers, while the spiral mode was found at low swirl numbers (Lucca-Negro and O’Doherty, 2001). Several theories have been proposed to explain the onset, internal structure and mode selection of vortex breakdown. In the wave theories proposed by Squire (1960) and Benjamin (1962), the abruptness of vortex breakdown indicates the existence of a critical state. In supercritical flows, disturbances are propagating downstream. In subcritical flows, standing waves can exist and the disturbances propagate upstream and downstream and cause vortex breakdown.

The role of hydrodynamic instabilities on vortex breakdown was also investigated by several researchers. Jones (1960) indicated that a Rankine vortex is unstable only to spiral disturbance and that a Hall vortex, with constant axial velocity, is stable to axisymmetric disturbances. Later, Lessen et al. (1974) performed a linear inviscid stability analysis of swirling flows by considering different modes of disturbance. Their results indicated that for small swirl parameter $q$ (which relates to the ratio of the magnitude of maximum swirl velocity to axial velocity), the disturbances die out quickly if $n = 1$ ($n$ is the azimuthal wave number). However, for negative values of $n$, the amplification rate increases, and then decreases. Although the above theories improve our understanding of vortex breakdown, none can completely and accurately describe all of the features of the vortex breakdown (Lucca-Negro and O’Doherty, 2001).
Numerical simulations of swirling flows were restricted to steady state calculations before 1998, primarily to emphasize the swirl effect on the size of the recirculation zone. A summary of experimental and numerical research of swirl flow was given by Sung (1999). Sloan et al. (1986) suggested that the eddy viscosity based on standard $k-\varepsilon$ model was inherently inadequate and necessitated a redistribution of stress magnitudes. Large Eddy Simulation (LES) turbulence models were just starting to be applied to swirl flow to analyze and visualize vortex breakdown phenomena. Pierce and Moin (1998) found that the confined swirling flow could be very sensitive to downstream boundary conditions, as suggested by Chao et al. (1991). Kim et al. (1999) investigated a swirl-stabilized gas-turbine combustor flow. A complex vortex shedding pattern with significant azimuthal structures was clearly identified. Both of these previous studies showed that LES could be useful in the study of the characteristics of swirling flow, such as vortex breakdown and PVC.

The discussion in the previous sections describes, in essence, the fundamentals of combustion instability as they relate to a lean-premixed swirl-stabilized combustor. With this overall understanding of the basic features of combustion instabilities, the approaches in modeling combustion dynamics are presented in the next sections.

### 1.2.5 Analytical Modeling of Heat Release Response

Even though combustion instability is one of the most difficult physical phenomena to model, some analytical models (Crocco and Cheng, 1956; Dowling, 1999; You et al., 2003a) have been developed that qualitatively describe the important phenomena. In many of these models, establishing a relationship between the heat release fluctuation and the pressure fluctuation is essential. However, as stated in previous sections, various physical processes, such as flame surface variations, equivalence ratio fluctuation, vortex shedding, are involved in
combustion instability and none of these processes can be modeled in sufficient detail. Usually, the heat release to pressure oscillation can be represented using a simple two-parameter representation defined below:

$$\hat{R}_p = \frac{\hat{q} / \hat{q}}{\hat{p} / \bar{p}}$$  \hspace{1cm} (1.7)

The heat release factor $\hat{R}_p$, which is a complex variable giving the magnitude and phase difference between pressure and heat release fluctuations, has to be determined for the specific problem and frequency in question.

One of the commonly used combustion response models is the time lag model, which was extensively used in the early literature to describe combustion instabilities in rocket motors (Crocco and Cheng, 1956). Basically, the time lag model tries to qualitatively explain the existence of the relationship between fuel injection and combustion for sustaining combustion instability. The time lag model can be briefly summarized as follows (Culick, 1988). Suppose that at time $t$, the pressure in the chamber suddenly decreases, causing an increase in the flow of fuel through the injector. The increased mass is convected downstream to the flame front and burns at some later time $t + \tau$, where $\tau$ is the time lag. The time scales that contribute to the time lag are the convection time needed to travel the distance from the fuel injection location to the flame front, the mixing time for fresh air and fuel mixture mixed with hot product gases, and the chemical time corresponding to the ignition delay. If the pressure in the chamber is increasing when the added fuel burns, the energy release tends to encourage the increase in pressure. A quantitative expression relating the fuel burning rate $\dot{m}_b$ to the injection rate $\dot{m}_i$ can be derived as:

$$\dot{m}_b(t) = \dot{m}_i(t - \tau)(1 - d\tau / dt)$$  \hspace{1cm} (1.8)
In the above equation, the mass burning flow rate at time, \( t \), can be given by the fuel mass flow rate injected at an earlier time, \( t - \tau \). Assuming the time lag \( \tau \) is constant and independent of local thermodynamic properties, Eq. 1.8 becomes:

\[
\dot{m}_b(t) = \dot{m}_i(t - \tau)
\]  \hspace{1cm} (1.9)

The assumption that the time lag is constant usually is not valid. To derive an equation for the rate of change in the time lag, one usually considers the process of the conversion of fuel into combustion products. Many models assume that the time lag is only sensitive to the pressure and let \( f(p) \) designate a function that globally describes this conversion process. Then an expression for \( d\tau / dt \) can be obtained as:

\[
1 - d\tau / dt = 1 + n [p'(t) / \bar{p} - p'(t - \tau) / \bar{p}]
\]  \hspace{1cm} (1.10)

where \( n \) is the interaction index given by \( n = \partial(\ln f) / \partial(\ln p) \). After some manipulations, the basic result of the time lag theory can be obtained as:

\[
\dot{m}_b'(t) = \overline{m}_b n [p'(t) / \bar{p} - p'(t - \tau) / \bar{p}]
\]  \hspace{1cm} (1.11)

Heat release fluctuations can be expressed by a similar expression:

\[
\hat{q}'(t) = \hat{q} n [p'(t) / \bar{p} - p'(t - \tau) / \bar{p}]
\]  \hspace{1cm} (1.12)

or

\[
\hat{q} / \bar{q} = n [1 - e^{-\lambda t}] \hat{\rho} / \bar{\rho}
\]  \hspace{1cm} (1.13)

Obviously, such a two-parameter representation is an enormous simplification of the real situation. The time lag model has many difficulties in explaining and predicting combustion
instability phenomena associated with nonlinear processes. Even with its shortcomings, the model has the capability of explaining qualitatively the interaction between the fuel supply system and the combustion chamber. Recently, the time lag model was applied to the study of combustion dynamics in lean premixed combustors by Richards and Janus (1997) and by Lieuwen and Zinn (1998a, b). Effects of fuel line length and inlet acoustical boundary conditions were incorporated into the development of their time lag model (Lieuwen and Zinn, 1998a).

A more sophisticated heat-release response model was recently proposed by Fleifil et al. (1996). The model treats the flame surface evolution equation and the heat release is determined from flame surface area per volume and the flame speed. Their results give the response of a laminar-premixed flame to flow oscillations. After correlating with the time lag model, the time-lag between the unsteady heat release and velocity perturbation was found to be a function of burning velocity and it increased as the burning velocity decreased. Later, their work was extended by Dowling (1999) under turbulent conditions by using a time-invariant turbulent flame speed to model the turbulent flame surface evolution. Her investigation of linear fluctuations showed that the transfer function between heat release and velocity determined analytically from their model agrees with the experimental data from Bloxisidge et al. (1988). For nonlinear fluctuations, the predicted flame front undergoes significant distortion as seen in Schlieren films.

Peracchio and Proscia (1999) extended the previously published works and proposed a more comprehensive heat release/acoustic model on a single nozzle rig (SNR), which considered both equivalence ratio and flame surfaces area fluctuations as sources of heat-release fluctuations. The effect of equivalence ratio was included using time-lag concepts and the dynamics of flame surface area were described using the flame model proposed by Fleifil et al. (1996). The resultant model’s performance was verified using experimental data.
1.2.6 Numerical Modeling of Turbulent Combustion Dynamics

Turbulence remains a challenge in fluid mechanics due to its strong nonlinear behavior, although the topic has been studied for more than one hundred years. Numerical simulation of turbulent motions may be classified into three categories: direct numerical simulation (DNS), Large eddy simulation (LES), and Reynolds-averaged Navier-Stokes Simulation (RANS). RANS has been used for many engineering applications. Large-eddy-simulation techniques may be viewed as the next step in addressing fluid mechanics problems where RANS failed to deliver accurate results and the computer power requirement of DNS for solving engineering problems far exceeds our current computer capabilities. The techniques of LES compute the contributions of large energy-carrying structures to mass, momentum, and energy transfer, with the effect of small-scale turbulence modeled either analytically or empirically. They are most suited for the study of gas turbine combustion dynamics, since the flow field of concern is highly unsteady and dominated by turbulence motions that can be adequately resolved computationally.

1.2.6.1 Large Eddy Simulation (LES)

One of the characteristics of turbulent flow is that various length scales exist in the global structure, and each length scale functions differently among them. While large-scale eddies transfer the kinetic energy of the mean flow to turbulent kinetic energy, small-scale eddies dissipate turbulent kinetic energy to internal energy. Large-scale eddies are strongly dependent on mean flow and geometry, and small-scale eddies tend to be more homogeneous and universal, and less affected by the boundary conditions. In LES, the contribution of the large energy-carrying structures to momentum, and energy transfer are computed accurately, and only the effect of the smallest scales of turbulence is modeled. Since the small scales tend to be more
homogeneous and universal, and less affected by boundary conditions, there is hope that models for their behavior can be simpler and require fewer adjustments when applied to different flows than similar models for RANS equations. The main role of the sub-grid scale (SGS) model is, therefore, to remove energy from the resolved scales, mimicking the drain of energy associated with the energy cascade. Most SGS models are eddy viscosity models: Smagorinsky’s model (1963), Erlebacher’s model (compressible flow version of the Smagorinsky model) (1992), Germano’s dynamic model for incompressible flows (1991), and the dynamic models for compressible flows (Ghosal et al., 1995). The assumption of an algebraic Smagorinsky-type model is that the equilibrium flow of turbulent energy cascade and model coefficients are determined from isotopic turbulence decay. Thus, ad hoc corrections such as wall functions or intermittency functions have been applied to tune the anisotropic flow properties near the boundary. The introduction of dynamic models circumvents this basic assumption and they are able to compute non-equilibrium flow by calculating model coefficients directly based on Germano’s (1991) identity. These dynamic models have demonstrated the possibility of the application of LES to a variety of flows in complex engineering geometries. However, the compressible version of the Smagorinsky model, along with the a damping function taking into account the inhomogeneities near the wall, is used in the present work because of its simplicity and reasonable computational cost.

Several attempts have been made to study combustion dynamics using LES. Menon and Jou (1991) conducted a pioneering two-dimensional LES of combustion dynamics in an axisymmetric ramjet combustor. Results captured globally the unstable flame evolution observed in experiments. Kailasanath et al. (1991) also investigated combustion dynamics in an axisymmetric ramjet combustor; heat release from chemical reactions is found to amplify the low-frequency oscillations observed in the non-reacting flow. Thibaut and Candel (1998) studied the flashback phenomenon in a backward-facing step configuration using a two-dimensional
analysis. The mechanism of flashback associated with combustion dynamics was investigated. Schonfeld and Poinsot (1999) studied the influences of initial and boundary conditions on premixed combustion instabilities in a gas-turbine burner. Kim et al. (1999) investigated a swirl-stabilized gas-turbine combustor flow. A complex vortex shedding pattern with significant azimuthal structures was clearly identified. Angelberger et al. (2000) conducted a two-dimensional simulation of a premixed dump combustor with acoustic forcing. Fureby (2000) investigated the combustion instabilities in a dump combustor and a model afterburner. Vortex shedding was found to be the main contributor to the driving of the combustion instabilities. Wang et al. (2003) recently examined the vortical flow dynamics in swirl-stabilized injectors with radial entry. Various flow instability mechanisms, including the Kelvin-Helmholtz, helical, and centrifugal instabilities as well as their mutual interactions, were investigated in detail.

1.2.6.2 LES Combustion Models for Premixed Turbulent Flame

In the treatment of turbulent reacting flows within the context of LES, detailed flame structures are often not resolved, and combustion models are needed at subgrid scales (SGS) (Candel et al., 1999). Modeling of the SGS reaction-rate term using the Arrhenius law based on filtered quantities (i.e., no SGS combustion model) often under-predicts the global turbulent burning rate (since the unresolved flame is wrinkled at scales below the LES resolution, which typically increases the global reaction rate (Charlette, 2002), and thus may lead to unexpected flame blow-off (Boger et al., 1998). Table 1-1 summarizes a variety of approaches that have recently been employed to perform LES of premixed turbulent combustion. These models can be broadly classified into two categories: flamelet and non-flamelet models. Flamelet models, such as the flame surface density-approach, flame-wrinkling model and level-set model, generally assume chemical reactions to be confined in a thin, sheet-like laminar flame structure whose inner
layer is unaffected by turbulence, a situation that occurs in many combustion systems (Peters, 2000; Hawkes, 2001). In the following, the combustion models listed in Table 1-1 are briefly reviewed.

Eddy-break-up type models usually assume that the fuel reaction rate is controlled by a characteristic turbulent time scale (Candel et al., 1999), although a chemical time scale can be included (Furbey and Lofstrom, 1994; Furbey and Moller, 1995; Moller et al., 1996). The models often tend to over-estimate the reaction rate within the context of RANS. For LES, the model constants seem to be strongly dependent on flow conditions and numerical mesh size (Candel et al., 1999; Furbey and Lofstrom, 1994). In thickened-flame models (Thibaut et al., 1998; Angelberger et al., 2000; Charlette et al., 2002; Colin et al., 2000) the flame is artificially broadened by increasing the thermal diffusivity, while keeping the flame propagation properties (i.e., flame speed) unchanged by reducing the reaction rate. The resultant thickened flame can thus be resolved on the LES grid using the Arrhenius law. Thickened-flame models are widely used because of their capability of treating complex chemistry and transient phenomena such as ignition, extinction, and flame-wall interaction. However, as indicated by Colin et al. (2000) the Damkohler number (defined as the ratio of turbulent time scale to chemical time scale) is changed in this approach. The ensuing modification of the flame response to turbulent motions may introduce some unknown effects in the simulation of combustion dynamics.

In the linear eddy model (Chakravarthy and Menon, 2000; Chakravarthy and Menon, 2001), the large-scale, resolvable scalar processes are simulated explicitly on the LES grid, while SGS turbulent processes and chemical reactions occurring within each numerical cell are treated using a one-dimensional model. This approach is complex and could be time-consuming since the one-dimensional model is used in each cell and the advection of scalars between LES cells requires additional treatment. In the flame surface-density approach (Boger, 1998; Hawkes and Cant, 2000; Hawkes and Cant, 2001), flame-wrinkling model (Weller et al., 1998; Furbey, 2000),
and turbulent flame-speed closure model (Flohr and Pitsch, 2000), a filtered progress variable is usually solved. The unclosed reaction source term is modeled by introducing a SGS flame-surface density, a SGS flame-wrinkling factor (defined as the ratio of the SGS flame surface area to its projection in the propagation direction) or a SGS turbulent flame speed, respectively. The first two parameters can be obtained from either an algebraic expression (Charlette et al., 2002a, 2002b; Boger et al., 1998) or a balance equation (Hawkes and Cant, 2000), while the last parameter comes from existing theoretical and experimental data for turbulent flame speed. In general, modeling of these three terms is closely related to flame wrinkling effects caused by unsolved turbulent motions.

The G-equation approach attempts to describe the premixed turbulent combustion from a geometrical point of view. The flame front is represented by an arbitrary iso-surface $G_0$ in a scalar field $G$ whose evolution is formulated using the so-called G-equation. Since the G-field outside the flame front is not uniquely defined, several approaches can be used. Menon and his colleagues (Menon and Jou, 1991; Kim et al., 1999) regarded G as a progress variable (i.e., $G=0$ and 1 for the fresh unburnt and burnt gases, respectively). The model is simple and easy to implement, but the numerical difficulties and grid resolution may incorrectly broaden the flame (Menon and Jou, 1991; Kim et al., 1999). Peters (2000), on the other hand, proposed a level-set approach that defines $G$ as a distance function outside the flame front, where the flame front position is given by $G = 0$. This approach, along with a laminar flamelet library and a presumed PDF method, offers a more realistic treatment of premixed turbulent flame dynamics. Another advantage of the level-set approach is that chemistry is decoupled computationally from turbulence and the difficulty of modeling turbulent chemical reaction rates can thus be avoided.

The level-set approach has been extensively explored by Peters in his monograph (2000) and tested by Herrmann (2000) and Bai and Nilsson (2001) within the context of RANS. Its
application to LES seems promising and has recently received substantial attention (Duchamp and Pitsch, 2000; Pitsch and Duchamp, 2002). It will be implemented in the present study.

1.3 Outline of Thesis

The present work attempts to model the unsteady combustion dynamics in model lean-premixed gas-turbine combustors. The specific objectives are to (1) develop and implement a level-set flamelet library approach for the numerical treatment of premixed turbulent flames in the context of LES, (2) numerically and systematically investigate combustion dynamics in a LPM swirl-stabilized combustor with a single swirl injector, and (3) develop an analytical model of premixed turbulent flame response to flow oscillations for the purpose of prediction and control of combustion instabilities.

In chapter 2, the energy transfer mechanisms among mean flow motions, periodic motions, and background turbulent motions in turbulent reacting flows are investigated using a triple decomposition technique. In particular, the Rayleigh criterion, which has been used in many qualitative descriptions of combustion instabilities, and formerly been derived using Reynolds decompositions, is revisited.

Chapter 3 gives a detailed discussion of the theoretical formulation. The analysis is based on the complete conservation equations of mass, momentum, energy, and species concentration, with consideration of finite-rate chemical reactions and variable thermophysics properties. Turbulent closure is achieved using the Large-Eddy-Simulation technique. The compressible-flow version of the Smagorinsky model was employed to describe subgrid-scale turbulent motions and the effect on large-scale structures. A recently developed level-set flamelet library approach is used to simulate premixed turbulent combustion. In this model, the flame front is represented by an arbitrary iso-surface $G_0$ in a scale field $G$ whose evolution is
formulated using the so-called $G$-equation. Outside the flame front, $G$ is defined as a distance function. This approach, along with a laminar flamelet library and presumed PDF method, offers a more realistic treatment of premixed turbulent combustion.

In chapter 4, the governing systems are discretized using a density-based, finite volume methodology. The spatial discretization employs a second-order, central-differencing scheme in generalized coordinates. A fourth-order matrix dissipation model with a total-variation-diminishing (TVD) switch is employed to ensure computational stability and to prevent numerical oscillations in regions with steep gradients. Temporal discretization is obtained using a four-step Runge-Kutta integration scheme. A multi-block domain decomposition technique along with static load balance is used to facilitate the implementation of parallel computation with message passing interface at the domain boundaries. Various types of boundary conditions for the governing equations are discussed in detail.

In chapters 5 and 6, the theoretical and numerical framework described above is applied to investigate the unsteady combustion dynamics in a model gas-turbine combustor operated at Penn State. The stable flame dynamics and the bifurcation of flame structure from a stable to an unstable state were first investigated. It is found that the inlet air temperature and equivalence ratio are the two most important variables determining the stability characteristics of the combustor. The lean-premixed system operating in an unstable mode is also carefully studied, with emphasis on physical processes responsible for driving combustion instabilities.

In chapter 7, an analytical model, based on the level-set flamelet model and triple decomposition technique, is developed to model the combustion response of turbulent premixed flames to acoustic oscillations. The resultant combustion response model is incorporated into a three-dimensional acoustic analysis to investigate the stabilities characteristic of a swirl-stabilized combustor.
Table 1-1: Survey of LES Combustion Models for Premixed Turbulent Flame

<table>
<thead>
<tr>
<th>Model description</th>
<th>Application</th>
<th>References</th>
<th>Remarks</th>
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</thead>
<tbody>
<tr>
<td>Eddy-break-up type model</td>
<td>triangular-shaped bluff body</td>
<td>Fureby and Lofstrom, 1994; Fureby and Moller, 1995; Moller et al., 1996</td>
<td>filtered reaction rate determined by Subgrid-scale mixing and chemical kinetics</td>
</tr>
<tr>
<td>Thickened-flame model</td>
<td>backward facing step; premixed dump combustor; premixed flame in decaying isotropic turbulent flow</td>
<td>Thibaut and Candel, 1998; Angelberger et al., 2000; Charlette, etc., 2002a,b; Colin et al., 2000</td>
<td>Arrhenius law used for artificially thickened flame</td>
</tr>
<tr>
<td>Linear-eddy model</td>
<td>turbulent stagnation point premixed flame</td>
<td>Chakravarthy and Menson, 2000, 2001</td>
<td>small-scale turbulence and chemical process treated using a one-dimensional model</td>
</tr>
<tr>
<td>Flame surface-density approach</td>
<td>freely propagating turbulent premixed flame</td>
<td>Hawkes and Cant, 2000, 2001</td>
<td>filtered reaction rate modeled by introducing flame surface density</td>
</tr>
<tr>
<td>Flame-wrinkling model</td>
<td>rearward-facing step; triangular-shaped bluff body</td>
<td>Weller et al., 1998; Fureby, 2000</td>
<td>filtered reaction rate estimated using flame wrinkling factor</td>
</tr>
<tr>
<td>Turbulent flame-speed closure model</td>
<td>backward-face step combustor.</td>
<td>Flohr and Pitsch, 2002</td>
<td>turbulent flame speed used to model filtered reaction term</td>
</tr>
<tr>
<td>G-equation model based on progress variable</td>
<td>swirl-stabilized gas-turbine combustor</td>
<td>Kim et al., 2000</td>
<td>flame front evolution described using G-equation based on progress variable</td>
</tr>
<tr>
<td>Level-set approach</td>
<td>turbulent Bunsen burner</td>
<td>Duchamp de Lageneste and Pitsch, 2000</td>
<td>flame front evolution governed by a level-set equation</td>
</tr>
</tbody>
</table>
Chapter 2

Energy Transfer Mechanism in Non-Reacting and Reacting Turbulent Flows

2.1 Introduction

It has been recognized for a long time that both random and periodic elements (or coherent structures) exist in a practical turbulent flow field. The imposed periodic fluctuations give rise to additional mechanisms of energy transfer between the mean and the background turbulent flow. The triple decomposition technique, in which flow variables are expressed as the sum of mean, periodic and turbulent components, is usually used to study coherent structures in turbulent flows (Hussain and Reynolds, 1970; Reynolds and Hussain, 1972). The equation for the mean flow motion is derived using time averaging, while the equation for the periodic motion is derived using ensemble phase averaging. In using the triple decomposition technique, the periodic motion itself and the interaction between the periodic motion and background turbulent field can be treated more specifically. Recently, triple decomposition was used by Reau and Tumin (2002) to develop a model for harmonic perturbations in turbulent wakes. It was also adopted by Apte and Yang (2002) to study unsteady flow evolution in porous chamber with forced acoustic excitation. The objective of this chapter is to investigate the energy transfer mechanism among mean flow motions, periodic motions and background turbulent motions for incompressible non-reacting flow and compressible reacting flows. In particular, the Rayleigh criterion, which has been used in many qualitative descriptions of combustion instabilities, and formerly was derived using Reynolds decomposition (in which the flow variable is decomposed as mean and fluctuation parts), is revisited using the triple decomposition technique.
2.2 Energy Transfer Mechanisms in Non-Reacting Turbulent Flow

2.2.1 Decomposition of Flow Variables

In a non-reacting turbulent flow investigation, the constant-properties assumption is usually used, since it makes the problem simpler and facilitates our analysis. In modeling non-constant-properties turbulent flows, it is generally assumed that the closure model derived for constant-properties flows can be easily extended to Favre-averaged equations (Jones, 1994).

Fig. 2-1 represents a typical pressure-time signal obtained from the porous chamber simulations by Apte and Yang (2002), including the mean, periodic, and turbulent motions. By following the triple decomposition technique of Hussain and Reynolds (1970) for incompressible flow, a flow variable can be expressed as the sum of the time-averaged $\overline{\mathcal{F}}(x)$, periodic $\mathcal{F}^p(x,t)$, and turbulent $\mathcal{F}'(x,t)$ quantities as follows:

$$\mathcal{F}(x,t) = \overline{\mathcal{F}}(x) + \mathcal{F}^p(x,t) + \mathcal{F}'(x,t)$$  \hspace{1cm} (2.1)
where the decomposition given above is based on the time averaging and ensemble phase averaging techniques. Two operations $\bar{}$ and $\langle \rangle$ are defined, where operation $\bar{}$ denote time averaging and operation $\langle \rangle$ denotes ensemble phase averaging, as below:

**Time averaging**

$$
\bar{\mathcal{F}}(x) = \left( \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \mathcal{F}(x, t_0 + n \Delta t) \right), \text{ where } N \Delta t >\tau >\Delta t
$$  \hspace{1cm} (2.2)

**Ensemble phase averaging**

$$
\langle \mathcal{F}(x,t) \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \mathcal{F}(x, t+n \tau)
$$  \hspace{1cm} (2.3)

$$
\langle \mathcal{F}(x,t) \rangle = \bar{\mathcal{F}}(x) + \mathcal{F}^a(x,t)
$$

where $\tau = 1/f$ is the period of oscillation. Some other useful properties that follow from the basic definition of time and ensemble phase averages are:

$$
< \mathcal{F} > = 0, \quad \bar{\mathcal{F}}^a = 0, \quad \bar{\mathcal{F}}^f = 0,
$$

$$
\bar{\mathcal{F}}_{\mathcal{R}} = \bar{\mathcal{F}}_{\mathcal{R}}, \quad < \mathcal{F}^a > = \mathcal{F}^a, \quad < \mathcal{F} > = \bar{\mathcal{F}} < \mathcal{R} >,
$$

$$
< \bar{\mathcal{F}} > = \bar{\mathcal{F}}, \quad < \mathcal{F}^a > = \mathcal{F}^a, \quad \bar{\mathcal{F}}^a < \mathcal{R}^f > = < \bar{\mathcal{F}}^a < \mathcal{R}^f > = 0.
$$  \hspace{1cm} (2.4)

The last relation states that the background turbulence and the periodic motions are uncorrelated on average. However, these two are not independent; periodic motions and background turbulent motions interact with each other (Hussain and Reynolds, 1970).

### 2.2.2 Dynamical Equations for Mean, Deterministic and Turbulent Motions in Non-Reacting Flows

The continuity and momentum equations for incompressible flows with constant properties are:
\[
\frac{\partial u_i}{\partial x_i} = 0 \quad \text{(2.5)}
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + v \frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad \text{(2.6)}
\]

Following the decomposition outlined above, we write velocity and pressure as:

\[
u_i = \overline{u}_i + u_i^a + u_i^t \quad \text{(2.7)}
\]

\[
p = \overline{p} + p^a + p^t
\]

Taking time averaging and ensemble phase averaging of the continuity equation, the component continuity equations are found to be:

\[
\frac{\partial \overline{u}_i}{\partial x_i} = 0, \quad \frac{\partial u_i^a}{\partial x_i} = 0, \quad \frac{\partial u_i^t}{\partial x_i} = 0. \quad \text{(2.8)}
\]

Substituting Eq. 2.7 and taking the time average of Eq. 2.6 gives the momentum equation for \( \overline{u}_i \):

\[
\overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{\partial}{\partial x_j} (\overline{u}_i^a u_j^a) - \frac{\partial}{\partial x_j} (u_i^a u_j^a) - \frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_i} + v \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} \quad \text{(2.9)}
\]

The momentum equation for \( u_i^a \) is derived by taking the ensemble phase average of the momentum Eq. 2.6 and subtracting Eq. 2.9:

\[
\frac{\partial u_i^a}{\partial t} + u_j \frac{\partial u_i^a}{\partial x_j} + u_j \frac{\partial u_i^a}{\partial x_j} = -\frac{\partial}{\partial x_j} (\overline{u}_i^a u_j^a) + \frac{\partial}{\partial x_j} (u_i^a u_j^a) - \frac{\partial}{\partial x_j} (\overline{u}_i^a u_j^a) - (\overline{u}_i^a u_j^a) + \overline{u}_i^a u_j^a
\]

\[
- \frac{1}{\rho} \frac{\partial \overline{p^a}}{\partial x_i} + v \frac{\partial^2 u_i^a}{\partial x_j \partial x_j} \quad \text{(2.10)}
\]

The momentum equation for \( u_i^t \) is derived by subtracting the ensemble phase averaged momentum equation Eq. 2.6 from itself:
In each of above the three equations, one term is unclosed and needs to be modeled. These terms, in fact, are three parts of the nonlinear term \(-u'_i u'_j\). The mean part of \(-u'_i u'_j\), which is the well-known Reynolds stress tensor, appears in Eq. 2.9. The periodic part, \((-<u'_i u'_j>-\overline{u'_i u'_j})\), can be found in Eq. 2.10. And the remaining non-periodic part, \((-u'_i u'_j-<u'_i u'_j>)\), is in Eq. 2.11. As we will see in the next section, the term, \(-\overline{u'_i u'_j}\), leads to the energy transfer between the mean and background turbulent flow field. The term, \(-\overline{(u'_i u'_j)^n}\), leads to the energy transfer between periodic motion and turbulent motion. The energy transfer between periodic motion and mean motion is caused by another term, \(-\overline{u'_i u'_j}\), which appears in both Eq. 2.9 and Eq. 2.10.

### 2.2.2 Energy Transfer Among the Mean, Deterministic, and Turbulent Flow Fields

In order to study the inter-component energy transport mechanisms, the equations for kinetic energies in the mean, deterministic, and turbulent flowfields can be derived as follows. Although energy equations are only manipulations of the momentum equations and do not introduce new information, they allow a clearer interpretation of the relationship between the various fields of flow, in terms of measurable quantities. Therefore, sets of kinetic-energy equations relating these three fields were developed in this study to describe the mean energy-transfer process.
The averaged kinetic energy per unit mass at a point is:

\[
\frac{1}{2} u_i u_i = \frac{1}{2} (\bar{u}_i + u_i^a + u_i'')(\bar{u}_i + u_i^a + u_i'')
\]

\[
= \frac{1}{2} \bar{u}_i \bar{u}_i + \frac{1}{2} u_i^a u_i^a + \frac{1}{2} u_i' u_i'
\]

Eq. 2.12 states that the total averaged kinetic energy can be divided into three parts: the kinetic energy of the mean flow, the kinetic energy of the periodic motions, and the kinetic energy of the background turbulent motions.

The equation for the kinetic energy of the mean flow \( \frac{1}{2} \bar{u}_i \bar{u}_i \) can be obtained by multiplying Eq. 2.9 by \( \bar{u}_i \):

\[
\bar{u}_j \frac{\partial}{\partial x_j} \left( \frac{\bar{u}_i \bar{u}_i}{2} \right) = u_i^a u_i^a \frac{\partial \bar{u}_i}{\partial x_j} + u_i^a u_j' \frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial}{\partial x_j} (\bar{u}_i (u_i^a u_i^a + u_i' u_j'))
\]

\[
- \frac{\bar{u}_i}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (v \bar{u}_i \frac{\partial \bar{u}_i}{\partial x_j}) - v \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j}
\]

The equation for the kinetic energy of the periodic motion \( \frac{1}{2} u_i^a u_i^a \) can be obtained by multiplying Eq. 2.10 by \( u_i^a \) and taking the time average:

\[
\frac{\partial}{\partial t} \left( \frac{u_i^a u_i^a}{2} \right) + \bar{u}_j \frac{\partial}{\partial x_j} \left( \frac{u_i^a u_i^a}{2} \right) + u_j^a \frac{\partial}{\partial x_j} \left( \frac{u_i^a u_i^a}{2} \right) = -u_i^a u_j' \frac{\partial \bar{u}_i}{\partial x_j} + (u_i^a u_i')' \frac{\partial \bar{u}_i}{\partial x_j}
\]

\[
- \frac{\partial}{\partial x_j} u_i^a (u_i^a u_j')' - \frac{u_i^a}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (v u_i^a \frac{\partial \bar{u}_i}{\partial x_j}) - v \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j}
\]

The equation for the kinetic energy of the turbulent motion \( \frac{1}{2} u_i' u_i' \) can be obtained by multiplying Eq. 2.11 by \( u_i' \) and taking the time average:
Each of the time-averaged equations for the mean, deterministic, and turbulent energies contains the convection, production, pressure work, and dissipation terms. The production and dissipation terms are of particular interest in understanding energy exchange among the three constituent flowfields. Several important points are noted here.

First, the term \( u'_i u'_j \partial \bar{u}_i / \partial x_j \) appears, with opposite signs, in Eq. 2.13 and Eq. 2.15. It serves as a pathway in the exchange of kinetic energy between the mean and turbulent fields. This term represents the primary production mechanism in stationary flows.

Second, the term \( u'_a u'_j \partial \bar{u}_i / \partial x_j \), which appears in both Eq. 2.13 and Eq. 2.14, but with opposite signs, represents the product of the mean shear and the mean correlation between components of deterministic velocity. It characterizes the energy transfer between the mean and deterministic fields.

Third, mean kinetic energy is exchanged between the deterministic and turbulent fields, as characterized by the term \( (u'_i u'_j)^a \partial \bar{u}_i^a / \partial x_j \), which appears in both Eq. 2.14 and Eq. 2.15. Its negative sign in Eq. 2.15 represents the production of turbulent kinetic energy due to periodic motions. Its positive sign in Eq. 2.14 represents a sink for the kinetic energy of periodic motions.

Finally, each of the time-averaged equations for the mean, deterministic, and turbulent energies contains a dissipation term. These terms are, \( \nu \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j} \), \( \nu \frac{\partial \bar{u}_i^a}{\partial x_j} \frac{\partial \bar{u}_i^a}{\partial x_j} \) and \( \nu \frac{\partial \bar{u}_i^a}{\partial x_j} \frac{\partial \bar{u}_i^a}{\partial x_j} \), which can be found in the thermal energy equation Eq. 2.16. The dissipations by the mean and
periodic motions are expected to be much smaller than the turbulent dissipation from dimensional analysis.

\[
\frac{\partial (c_i T)}{\partial t} + \frac{\partial (u_j c_i T)}{\partial x_j} = -\frac{\partial (c_i u_j^\prime T^\prime)}{\partial x_j} - \frac{\partial (c_i u_j^\prime T^\prime)}{\partial x_j} - \frac{1}{\rho} \frac{\partial q_i}{\partial x_i} \\
+ \nu \frac{\partial u_i^\prime}{\partial x_j} \frac{\partial u_i^\prime}{\partial x_j} + \nu \frac{\partial u_i^a \partial u_i^a}{\partial x_j} + \nu \frac{\partial u_i^l \partial u_i^l}{\partial x_j} \frac{\partial u_i^l}{\partial x_j} \frac{\partial u_i^l}{\partial x_j}
\]

(2.16)

where \( q_i = -\lambda \partial T / \partial x_i \).

The energy exchange among the mean, periodic, and turbulent flow fields can be summarized by the schematic diagram shown in Fig. 2-2. The triple decomposition used in the present study leads to an additional pathway for the transfer of energy between the mean and turbulent motions through the deterministic unsteady motions.

Fig. 2-2: Energy exchange mechanisms among the mean, periodic, and turbulent motions in non-reacting turbulent flows
2.3 Energy Transfer Mechanisms in Compressible Reacting flows

2.3.1 Decomposition of Flow Variables in Reacting Flows

The triple decomposition technique for incompressible flow is extended to include compressibility effects using Favre-averaged (or density-weighted) time and ensemble phase averaging techniques (given hereafter). These averaging techniques offer mathematical simplification and eliminate triple correlations between the density and velocity fluctuations in compressible flows. Accordingly, the flow variables (except for density and pressure) can be expressed as the sum of the density-weighted time-averaged, periodic, and turbulent quantities as follows:

\[
\mathcal{Z}(x,t) = \tilde{\mathcal{Z}}(x) + \bar{\mathcal{Z}}^p(x,t) + \bar{\mathcal{Z}}^l(x,t)
\]  

\(2.17\)

Here \(\leftrightarrow\), \(\bar{\cdot}\) and \(\bar{\cdot}\) are used to represent density weighted time averaged, periodic and turbulent quantities. Two operations \(\bar{\cdot}\) and \(\leftrightarrow\) are defined, where the operation \(\bar{\cdot}\) denotes time averaging and the operation \(\leftrightarrow\) denotes ensemble phase averaging. Density-weighted time and ensemble phase averaged variables are defined as follows:

Density weighted time averaging

\[
\tilde{\mathcal{Z}}(x) = \rho \frac{\mathcal{Z}(x)}{\rho}
\]

\[
\bar{\mathcal{Z}}(x) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \rho \mathcal{Z}(x,t_0 + n \Delta t)
\]

\(2.18\)

Density weighted ensemble phase averaging
\[
\bar{\mathcal{F}}(x) + \bar{\mathcal{F}}(x,t) = \langle \rho \mathcal{F}(x,t) \rangle / \rho < \rho >
\]

\[
\langle \rho \mathcal{F}(x,t) \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \rho \mathcal{F}(x,t+n T)
\]  

so that

\[
\bar{\mathcal{F}}(x,t) = \frac{\langle \rho \mathcal{F}(x,t) \rangle}{\rho} - \frac{\rho \bar{\mathcal{F}}(x)}{\rho}
\]

\[
(\rho \mathcal{F})^a = \langle \rho \mathcal{F} - \bar{\rho} \mathcal{F} \rangle = \rho^a \bar{\mathcal{F}} + \rho^a \bar{\mathcal{F}}
\]

where \( T \) is the period of oscillation. \( \bar{\mathcal{F}}(x) \) is the density-weighted time average starting from the initial time \( t_0 \), after which steady fluctuations of flow properties are observed. \( \bar{\mathcal{F}}(x,t) \) is the density-weighted phase average and represents the periodically fluctuating part. Some other useful properties that follow from the basic definition of time and ensemble phase averages are:

\[
\bar{\rho} \langle \bar{\mathcal{F}} + \bar{\mathcal{F}}^i \rangle = 0, \quad < \rho \mathcal{F}^i >= 0, \quad \bar{\mathcal{F}}^i \neq 0
\]

\[
\bar{\mathcal{F}} \mathcal{R} = \bar{\mathcal{F}} \mathcal{R}, \quad < \mathcal{F}^i \mathcal{R} >= \bar{\mathcal{F}}^i < \mathcal{R} >, \quad < \bar{\mathcal{F}} \mathcal{R} >= \bar{\mathcal{F}} < \mathcal{R} >.
\]  

\[
< \bar{\mathcal{F}} >= \bar{\mathcal{F}}, \quad < \mathcal{F}^i >= \bar{\mathcal{F}}^i, \quad \rho \bar{\mathcal{F}}^i \mathcal{R}^i = \langle \rho \mathcal{F}^i \mathcal{R}^i \rangle = 0.
\]  

The last relation states that the density weighted background turbulence and the periodic motions are uncorrelated on average.

### 2.3.2 Governing Equations for Reacting Flows

The equations for motion in the mean, deterministic, and turbulent flowfields can be obtained by applying the decomposition and average techniques defined above to the basic governing equations for reacting flow. The mass, momentum, energy and species conservations for reacting flows are:

\[ \text{Mass Conservation} \]

\[ \text{Momentum Conservation} \]

\[ \text{Energy Conservation} \]

\[ \text{Species Conservation} \]
\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0
\]  
(2.22)

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}
\]  
(2.23)

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_j E}{\partial x_j} = -\frac{\partial q_i}{\partial x_i} - \frac{\partial u_j p}{\partial x_j} + \frac{\partial u_j \sigma_{ij}}{\partial x_j}
\]  
(2.24)

\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = \omega_k - \frac{\partial \rho U_{k,j} Y_k}{\partial x_j}, \quad k = 1, \ldots, N
\]  
(2.25)

where

\[
\sigma_{ij} = -\frac{2}{3} \mu \frac{\partial u_i}{\partial x_j} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]  
(2.26)

\[
E = e + \frac{u_i u_i}{2} = h - \frac{P}{\rho} + \frac{u_i u_i}{2} = c_i T + \frac{u_i u_i}{2}
\]  
(2.27)

\[
h = \sum_{k=1}^{N} Y_k h_k = \sum_{k=1}^{N} Y_k \left( \Delta h_{j,k} + \int_{h_i}^{h_{j,k}} c_{p,k} (T') dT' \right)
\]  
(2.28)

\[
q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^{N} h_k Y_k U_{k,i}
\]  
(2.29)

\[
p = \rho R T = \rho R u_i \sum_{k=1}^{N} \frac{Y_k}{W_k}
\]  
(2.30)

Also, the global conservation of mass requires that:

\[
\sum_{k=1}^{N} \omega_k = 0 \quad \text{and} \quad \sum_{k=1}^{N} \rho Y_k U_{k,j} = 0
\]  
(2.31)

where \( U_{k,j} \) represents the diffusion velocity of species \( k \).
Combine the momentum equation, energy equation and species equation. An equation for temperature can be obtained as follows:

\[
\rho c_p \left( \frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} \right) = \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) + \left( \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} \right) + \sigma_{ij} \frac{\partial u_j}{\partial x_j} - \sum_{k=1}^{N} h_k \omega_k 
\]

\[
+ \sum_{k=1}^{N} \rho U_{k,j} c_{p,k} \frac{\partial T}{\partial x_i} \tag{2.32}
\]

Assume that all of the specific heats for all species are equal \( c_{p,k} = c_p \). Then the last term in Eq. 2.32 disappears.

\[
\rho c_p \left( \frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} \right) = \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) + \left( \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} \right) + \sigma_{ij} \frac{\partial u_j}{\partial x_j} - \sum_{k=1}^{N} h_k \omega_k \tag{2.33}
\]

To simplify our analysis, we further assume that some properties such as \( R, \gamma, c_p, c_v \) are constant and we denote the heat release term as \( \dot{q} = -\sum_{k=1}^{N} h_k \omega_k \) and the dissipation term as \( \Phi = \sigma_{ij} \frac{\partial u_j}{\partial x_j} \). Then Eq. 2.33 can be written as:

\[
\frac{\partial \rho c_v T}{\partial t} + \frac{\partial \rho u_j c_v T}{\partial x_j} = \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) - p \frac{\partial u_j}{\partial x_j} + \Phi + \dot{q} \tag{2.34}
\]

This equation can also be written as

\[
\frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} = -p \frac{\partial u_j}{\partial x_j} + (\gamma - 1) \left( \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) + \Phi + \dot{q} \right) \tag{2.35}
\]

Only the velocity components and temperature will be averaged with density weighting to avoid correlations between density and velocity fluctuations.

\[
\bar{u}_i = \bar{u}_i + u_i^\prime + u_i^\ddprime
\]

\[
\bar{T} = \bar{T} + T^\prime + T^\ddprime \tag{2.36}
\]
The density, pressure and stresses are decomposed into the periodic, time-averaged and random fluctuations.

\[
\rho = \overline{\rho} + \rho^a + \rho^i \\
p = \overline{p} + p^a + p^i \\
\sigma_{ij} = \overline{\sigma}_{ij} + \sigma_{ij}^a + \sigma_{ij}^l
\]  \hspace{1cm} (2.37)

### 2.3.3 Governing Equation for Mean, Deterministic and Turbulent Motions

Substitute Eq. 2.36 and Eq. 2.37 into Eq. 2.22 and make use of the definition given above. The continuity equation for the mean, deterministic and turbulent flowfields is obtained:

\[
\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial (\overline{\rho} \overline{u}_j)}{\partial x_j} = 0 \hspace{1cm} (2.38)
\]

\[
\frac{\partial \rho^a}{\partial t} + \frac{\partial <\rho > u_j^a}{\partial x_j} = 0 \hspace{1cm} (2.39)
\]

\[
\frac{\partial \rho^l}{\partial t} + \frac{\partial (\rho > u_j^l + \rho^l u_j)}{\partial x_j} = 0 \hspace{1cm} (2.40)
\]

The momentum equation for mean flowfield can be obtained by applying the time average of Eq. 2.23:

\[
\frac{\partial (\overline{\rho} \overline{u}_j \overline{u}_j)}{\partial x_j} = - \frac{\partial (\overline{\rho} u_i^a u_j^a)}{\partial x_j} - \frac{\partial (\overline{\rho} u_i^l u_j^l)}{\partial x_j} - \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{\sigma}_{ij}}{\partial x_j} \hspace{1cm} (2.41)
\]

The momentum equation for \( u_i^a \) is derived by taking the ensemble phase average of momentum Eq. 2.23 and subtracting Eq. 2.41:
\[ <p> \frac{\partial u_i^a}{\partial t} + <p> \vec{u}_j \frac{\partial u_i^a}{\partial x_j} + <p> u_j^a \frac{\partial u_i^a}{\partial x_j} = -<p> u_j^a \frac{\partial \vec{u}_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left( (\rho u_i^a u_j^a) - \rho u_i^a u_j^a \right) - \frac{\partial p^a}{\partial x_i} + \frac{\partial \sigma_{ij}^a}{\partial x_j} - \rho \frac{\partial \mathcal{N}_{ui,j}^a}{\partial t} \right) \] (2.42)

where \[ \mathcal{N}_{ui,j}^a = -\frac{\partial (\rho u_i^a u_j^a)}{\partial x_j} - \frac{\partial (\rho u_i^a u_j^a)}{\partial x_j} - \frac{\partial p^a}{\partial x_i} + \frac{\partial \sigma_{ij}^a}{\partial x_j} \]

The momentum equation for \( u_i^j \) is derived by subtracting the ensemble phase averaged momentum equation Eq. 2.23 from itself:

\[ \rho \frac{\partial u_i^j}{\partial t} + \rho \left( \vec{u}_j + u_j^a \right) \frac{\partial u_i^j}{\partial x_j} = -\rho u_j^i \frac{\partial \vec{u}_i}{\partial x_j} - \rho u_j^i \frac{\partial u_i^a}{\partial x_j} + u_i^j \frac{\partial \rho u_i^j}{\partial x_j} \] (2.43)

where \[ \mathcal{N}_{ui,j}^j = -\frac{\partial <p> u_i^j u_j^j >}{\partial x_j} - \frac{\partial <p>}{\partial x_i} + \frac{\partial <\sigma_{ij}^j >}{\partial x_j} \]

Similarly, in the non-reacting flow, in each of the above three equations, one term is unclosed and needs to be modeled. These terms are three parts of the nonlinear term \(-\rho u_i^j u_j^j \). The mean component \(-\rho u_i^j u_j^j \), which is the Reynolds stress tensor and can lead to energy transfer between the mean and background turbulent flow fields, appears in mean Eq. 2.41. The periodic component, \(-\left( \rho u_i^j u_j^j \right)^a \), which leads to energy transfer between the periodic motion and turbulent motions, can be found in periodic Eq. 2.42. The remaining non-periodic component \(-\left( \rho u_i^j u_j^j \right)^j \) is in Eq. 2.43. The energy transfer between periodic motion and mean motion is caused by another term, \(-\rho u_i^a u_j^j \), which appears in both Eq. 2.41 and Eq. 2.42.
2.3.4 Energy Transfer Among Mean, Deterministic and Turbulent Flow Fields

For compressible flows, the density-weighted averaged kinetic energy per unit mass is defined as follows:

\[
\overline{k} = \frac{1}{2} \overline{u_i u_i} = \frac{1}{2} \frac{\rho_i u_i}{\bar{\rho}} \\
= \frac{1}{2\bar{\rho}} \rho(u_i + u_i^a + u_i^t)(\overline{u_i} + u_i^a + u_i^t) = \frac{1}{2\bar{\rho}} (\rho \overline{u_i u_i} + \rho u_i^a u_i^a + \rho u_i^t u_i^t) \quad (2.44)
\]

\[
= \frac{1}{2} \overline{u_i u_i} + \frac{1}{2} u_i^a u_i^a + \frac{1}{2} u_i^t u_i^t
\]

The equation for \( \frac{1}{2} \overline{u_i u_i} \) is formed by multiplying Eq. 2.41 by \( \overline{u_i} \):

\[
\frac{\partial}{\partial x_j} (\bar{\rho} u_j \overline{u_i u_i} / 2) = \bar{\rho} u_j^a u_j^a \frac{\partial \overline{u_i}}{\partial x_j} + \bar{\rho} u_j^t u_j^t \frac{\partial \overline{u_i}}{\partial x_j} \\
- \frac{\partial}{\partial x_j} (\bar{u}_i \rho u_i^a u_j + \bar{u}_i \rho u_i^t u_j) + \bar{p} \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_i} (\sigma_{ij} - \bar{p})}{\partial x_j} - \frac{\sigma_{ij}}{\partial x_j} \frac{\partial \overline{u_i}}{\partial x_j} \quad (2.45)
\]

The equation for \( \frac{1}{2} u_i^a u_i^a \) is similarly obtained by multiplying Eq. 2.42 by \( u_i^a \) and then taking time average to yield:

\[
\frac{\partial}{\partial t} \left( \frac{\rho u_i^a u_i^a}{2} \right) + \frac{\partial}{\partial x_j} \left( \bar{\rho} u_j^a u_i^a \right) = \rho u_i^a u_j^a \frac{\partial \overline{u_i}}{\partial x_j} + (\rho u_j^a u_j^a) \frac{\partial \overline{u_i}}{\partial x_j} \\
- \rho u_i^a u_j \frac{\partial u_i^a}{\partial x_j} \frac{\partial \overline{u_i}}{\partial x_j} = (\rho u_i^a u_j^a)^a - \frac{\partial u_i^a}{\partial x_j} \frac{\partial \overline{u_i}}{\partial x_j} - \frac{\partial \overline{u_i} u_i^a \sigma_{ij}}{\partial x_j} - \frac{\sigma_{ij} \frac{\partial u_i^a}{\partial x_j}}{\partial x_j} + \frac{u_i^a \rho \overline{a_{ij}}}{\bar{\rho}} \quad (2.46)
\]

In multiplying Eq. 2.43 by \( u_i^t \), and taking the time average, one can obtain:
Similarly, in the incompressible flow, each of the time-averaged equations for the mean, deterministic, and turbulent energies contains the convection, production, pressure work and dissipation terms. The term $\overline{\rho u_j^i u_j^i u_i^i / \partial x_j}$ serves as a pathway for exchanging the kinetic energy between the mean and turbulent fields. The term $\overline{\rho u_j^i u_j^i \partial u_i^i / \partial x_j}$ characterizes the energy transfer between the mean and deterministic fields and serves as a basis for explaining the phenomena of flow-turning loss and acoustic streaming. The former refers to the loss of acoustic energy to the mean flow due to misalignment between the acoustic and mean flow velocities. The latter describes the modification of the mean flowfield due to impressed periodic excitation. The mean kinetic energy exchange between the deterministic and turbulent fields is characterized by the term $\overline{(\rho u_j^i u_j^i) u_i^i / \partial x_j}$. The dissipation terms in each of the time-averaged equations for the mean, deterministic, and turbulent energies are $\sigma_g \partial u_i / \partial x_j$, $\sigma_g \partial u_i / \partial x_j$, and $\sigma_g \partial u_i / \partial x_j$.

2.3.5 Energy Transfer from Chemical Energy to Turbulent Flow Field

When triple decomposition is first applied to Eq. 2.30 (equation of state), we obtain (assuming $R$ is constant):

\[
\frac{\partial}{\partial t} \left( \overline{\rho u_j^i u_j^i / 2} \right) + \overline{\rho u_j^i u_j^i / \partial x_j} + \overline{\rho u_j^i u_j^i / \partial x_j} = -\overline{\rho u_j^i u_j^i} \frac{\partial u_j^i}{\partial x_j} - (\overline{\rho u_j^i u_j^i}) \frac{\partial u_j^i}{\partial x_j} - \overline{\rho u_j^i u_j^i} \frac{\partial u_j^i}{\partial x_j} - \overline{\rho u_j^i u_j^i} \frac{\partial u_j^i}{\partial x_j} - \overline{\rho u_j^i u_j^i} \frac{\partial u_j^i}{\partial x_j} = \overline{\rho N_{c,s}}
\]
The equation for mean flow field $\bar{T}$ can be obtained by applying the time average of Eq. 2.34:

$$\bar{p} = \rho R \bar{T} \tag{2.48}$$

$$p^a = R < \rho T > - R \bar{p} = R(\rho^a \bar{T} + < \rho > T^a) \tag{2.49}$$

The equation for mean flow field $\bar{T}$ can be obtained by applying the time average of Eq. 2.34:

$$\frac{\partial (\bar{\rho}c_i \bar{T}^i)}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_j c_i \bar{T}^i)}{\partial x_j} = - \frac{\partial (\bar{\rho} \bar{u}_j c_i \bar{T}^i)}{\partial x_j} - \frac{\partial (\bar{\rho} \bar{u}_j c_i \bar{T}^i)}{\partial x_j} \frac{\partial \bar{T}}{\partial x_j} - \frac{\partial \bar{T}}{\partial x_j} - p \frac{\partial \bar{u}_j}{\partial x_j} \tag{2.50}$$

$$+ \Phi + \bar{q}$$

In acoustic fields, the energy transported by acoustic waves through a fluid medium is the sum of two components: the kinetic energy $\frac{1}{2} \bar{\rho}(u')^2$ and the potential energy $\frac{1}{2} (p')^2 / \bar{\rho}c^2$.

Similarly, the energy related to the periodic motions $\bar{e}$ can be regarded as the sum of acoustic potential energy $\frac{(p^a)^2}{2 \bar{\rho}c^2}$ and acoustic kinetic energy $\frac{\bar{\rho} u_i^a u_i^a}{2}$.

The equation for acoustic potential energy $\bar{e}_p = \frac{(p^a)^2}{2 \bar{\rho}c^2}$ can be obtained starting from Eq. 2.35 using the density-weighted triple decomposition technique.

$$\frac{\partial}{\partial t} \left( \bar{\rho} \frac{(p^a)^2}{2 \bar{\rho}c^2} \right) + \bar{u}_j \frac{\partial}{\partial x_j} \left( \bar{\rho} \frac{(p^a)^2}{2 \bar{\rho}c^2} \right) + \bar{u}_j \frac{\partial}{\partial x_j} \left( \bar{\rho} \frac{(p^a)^2}{2 \bar{\rho}c^2} \right) = - p^a \frac{\partial u_i^a}{\partial x_i} - \frac{p^a u_i^a \bar{\rho}}{\bar{\rho}} \frac{\partial \bar{p}}{\partial x_i}$$

$$- \frac{(p^a)^2}{\bar{\rho}} \frac{\partial (\bar{u}_j + u_i^a)}{\partial x_j} - \frac{p^a}{\bar{\rho}} \frac{\partial}{\partial x_j} (\bar{p} R (\rho u_i^a T^i)^a) + \frac{(\gamma - 1)}{\bar{\rho}} \frac{p^a (\rho R T i)}{\bar{p}} \frac{\partial u_i^a}{\partial x_j} \tag{2.51}$$

$$+ \frac{(\gamma - 1)}{\bar{\rho}} \frac{p^a}{\bar{\rho}} \frac{\partial (\bar{u}_j + u_i^a)}{\partial x_j} (\bar{\rho} \frac{\partial \bar{T}}{\partial x_j} + \Phi^a) + \frac{(\gamma - 1)}{\bar{\rho}} \frac{p^a \bar{q}}{\bar{\rho}} - \frac{1}{2 \gamma} \frac{(p^a)^2}{\bar{\rho}} \bar{N}_p$$

where $\bar{N}_p = \frac{\partial \bar{p}}{\partial t} + (\bar{u}_j + u_i^a) \frac{\partial \bar{p}}{\partial x_j}$

The kinetic energy equation of $\bar{e}_k = \bar{\rho} u_i^a u_i^a / 2$ can be rewritten as:
Combining the above two equations, we obtain a time-averaged equation for the total acoustic energy, \( \overline{E} = \overline{E}_p + \overline{E}_k = (p^a)^2 / 2\overline{\rho}^2 + \overline{\rho u_i^a u_i^a} / 2 \),

\[
\frac{\partial \frac{\overline{\rho u_i^a u_i^a}}{2}}{\partial t} + \frac{\partial}{\partial x_j} \left( \frac{\overline{\rho u_i^a u_i^a}}{2} \right) - \rho \frac{\overline{u_i^a u_i^a}}{2} \frac{\partial \overline{\rho u_i^a u_i^a}}{\partial x_j} - \rho \overline{u_i^a u_i^a} \frac{\partial \overline{u_i^a u_i^a}}{\partial x_j} + (\rho u_i^a u_i^a)^a \overline{\frac{\partial u_i^a}{\partial x_j}} - \sigma_{ij} \overline{\frac{\partial u_i^a}{\partial x_j}} = \frac{\partial \overline{\rho u_i^a u_i^a}}{\partial x_j}
\]

The term \( \frac{\partial \overline{u_i^a u_i^a}}{\partial x_j} \) appears, with opposite signs, in Eq. 2.51 and Eq. 2.52. It serves as a pathway for energy exchange between the acoustic kinetic energy \( \overline{E}_k \) and the acoustic potential energy \( \overline{E}_p \). When \( p^a \) and \( \frac{\partial \overline{u_i^a u_i^a}}{\partial x_j} \) are in phase, kinetic energy extracts energy from potential acoustic energy; otherwise, kinetic energy feeds energy to acoustic potential energy. After Eq. 2.51 and Eq. 2.52 are combined, there is one term \( \overline{\frac{\partial u_i^a}{\partial x_j}} p^a / \partial x_j \) on the left hand side of
Eq. 2.53, which represents the convection of the acoustic energy flux \( u_j \partial_x a \). This term will vanish, upon integration over a large volume of the flow (assuming that the flowfield in the volume is a closed system). Hence it also represents the transport of acoustic energy within the flowfield.

The source term \( (\gamma - 1) \frac{\partial a}{\partial \tilde{\phi}} / \tilde{p} \) on the right hand side of Eq. 2.53 corresponds to the unsteady heat release in the reacting flows. Let \( \theta \) be the phase difference between pressure and heat release oscillations, \( (\gamma - 1) \frac{\partial a}{\partial \tilde{\phi}} / \tilde{p} = (\gamma - 1) \frac{\partial a}{\partial \tilde{\phi}} \cos \theta / \tilde{p} \). If pressure and heat release are in phase \( (-\pi/2 < \theta < \pi/2) \), this term is positive, and energy is supplied to the system. Otherwise, pressure and heat release are out of phase \( (\pi/2 < \theta < 3\pi/4) \), energy is subtracted from the system. This result is of course closely related to the Rayleigh criterion.

Unsteady heat transfer \( \partial / \partial x_j (\lambda \partial T / \partial x_j) \) and dissipation \( \Phi \) play same the important roles on driving flow oscillations as unsteady heat release. However, the role of dissipation \( \Phi \) in energy transfer is two-fold: it always turns the periodic energy into thermal energy, but when its oscillation is in phase with pressure oscillation, it also tends to increase periodic energy.

In conclusion, the acoustic motions can obtain energy from several sources. They can extract energy from mean flow; they can receive energy from chemical reactions; they can exchange energy with background turbulent motions; they also will be dissipated into thermal energy. When there are no chemical reactions, the major energy source for periodic motions is the mean flow. With combustion, heat release from chemical reactions is the major energy source for driving acoustic motions. The transfer of energy from chemical for chemical reactions only takes place when heat release oscillations are in phase with pressure oscillations.
Fig. 2-3: Energy exchange mechanisms among the mean, periodic, and turbulent motions in reacting flows
Chapter 3

Theoretical Formulation

3.1 Governing Equations

The theoretical formulation is based on the full conservation equations of mass, momentum, energy and species concentration in Cartesian coordinates:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad (3.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (3.2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \left[(\rho E + p)u_i \right]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} \quad (3.3)$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial (\rho Y_k u_j)}{\partial x_j} = \omega_k - \frac{\partial \rho Y_k U_{k,j}}{\partial x_j}, \quad k = 1, \ldots, N \quad (3.4)$$

where $i$, $j$, and $k$ are the spatial coordinate index, the dummy index to spatial coordinate, and the species index, respectively. $N$ is the total number of species. $Y_k$ and $U_{k,j}$ represent mass fraction and diffusion velocities of species $k$, respectively. The viscous stress tensor $\tau_{ij}$ for a Newtonian fluid (with Stokes assumption) and the heat flux vector $q_j$ are defined as:
where \( \mu \) and \( \lambda \) are the coefficients of viscosity and heat conductivity, respectively. Within the thermodynamic regime of the present concern, viscosity coefficient \( \mu \) and thermal conductivity \( \lambda \) can be represented by polynomial functions of temperature. The specific total energy \( E \) is given by:

\[
E = e + \frac{u_j u_j}{2}
\]  

(3.7)

The governing equations are supplemented with the equation of state for an ideal gas. Then the specific internal energy, \( e \), is obtained as:

\[
e = h - \frac{p}{\rho}
\]  

(3.8)

The species specific heat at constant pressure, \( C_{p,k} \), can be approximated by a polynomial function of temperature:

\[
C_{p,k} = \sum_{p=1}^{M} a_{k,p} T^{p-1}
\]  

(3.10)
The formulation is closed by an equation of state for a perfect mixture:

\[ p = \rho R_u T \sum_{k=1}^{N} \frac{Y_k}{W_k} = \rho RT \]  \hspace{1cm} (3.11)

where \( R_u \) is the universal gas constant and \( W_k \) is the molecular weight of species \( k \).

To obtain the expression for the chemical reaction term, consider an \( L \)-step reaction mechanism with \( N \) species, which can be written as:

\[ \sum_{k=1}^{N} \begin{array}{c} \nu_{ki}'X_k \\ \nu_{ki}''X_k \\ \end{array} \xleftrightarrow{\kappa_{ki}} \sum_{k=1}^{N} \begin{array}{c} \nu_{ki}'X_k \\ \nu_{ki}''X_k \\ \end{array} , \hspace{0.5cm} i = 1, 2, ..., L \]  \hspace{1cm} (3.12)

where \( \nu_{ki}' \) and \( \nu_{ki}'' \) are the stoichiometric coefficients on the reactants and products side for species \( k \) in the \( i^{th} \) reaction. \( X_k \) represents the chemical formula of species \( k \). \( k_{fi} \) and \( k_{bi} \) are the reaction rate constants of the forward and backward reactions, respectively. They may take the following form:

\[ k_i(T) = A_i T^b \exp\left(-\frac{E_i}{R_u T}\right) \]  \hspace{1cm} (3.13)

where \( A, b, \) and \( E_i \) are empirical parameters and \( E_i \) represents the activation energy of reaction \( i \).

The following relationship expresses the net production rate \( \dot{\omega} \) of each species in a multi-step mechanism:

\[ \dot{\omega}_k = W_k \sum_{i=1}^{L} \left( \nu_{ki}' - \nu_{ki}'' \right) \left[ \kappa_{fi} \prod_{k=1}^{N} [X_k]^{\nu_{ki}'} - \kappa_{bi} \prod_{k=1}^{N} [X_k]^{\nu_{ki}''} \right] , \hspace{0.5cm} k = 1, 2, ..., N \]  \hspace{1cm} (3.14)

where \( W_k \) and \([X_k]\) represent the molecular weight and molar concentration of species \( k \). Note that the expression for the net production rate, Eq. 3.14, is valid only for elementary reactions. Since some researchers may use a global kinetic mechanism, the exponents for molar concentrations may differ from their stoichiometric coefficients.
3.2 Turbulence Closure: Large Eddy Simulation

A large-eddy simulation (LES) technique is implemented in the present work for turbulence closure. One of the characteristics of turbulent flow is that various length scales exist in the global structure, and each length scale functions differently. In the LES technique, the contribution of the large energy-carrying structures to momentum, and energy transfer are computed accurately, and only the effect of the unresolved scales of the turbulence is modeled. Large-scale eddies transfer the kinetic energy of the mean flow to turbulent kinetic energy, while small-scale eddies dissipate turbulent kinetic energy to internal energy. Large-scale eddies are strongly dependent on mean flow and geometry, and small-scale eddies tend to be more homogeneous and universal, and less affected by the boundary conditions. Thus, in theory, the subgrid scale (SGS) model (referred to as the model of smaller scales less than the computational grid in LES) can be simpler and require fewer adjustments when applied to different flows than similar models for the Reynolds-averaged Navier-Stokes (RANS) equations (Piomelli, 1999).

3.2.1 Filtering Operations

In a large eddy simulation, filtering operations are used to separate the large-scale from the small-scale turbulent motions. A filtered (or resolved, or large-scale) variable is defined as:

$$\tilde{f}(x) = \int_{-\infty}^{\infty} f(x)G_f(x-x')dx'$$  \hspace{1cm} (3.15)
where \( G_f \) is the filter function and \( \int_{-\infty}^{\infty} G_f(x) dx = 1 \). Leonard (1974) indicated that if \( G_f \) is only a function of \( x - x' \), differentiation and the filtering operation could commute each other. The most commonly used filter functions are the Top-hat, Gaussian, and Cutoff filters.

The Top-hat filter is popularly employed in physical space and is defined as:

\[
G_f(x) = \begin{cases} 
\frac{1}{\Delta} & \text{if } |x| \leq \Delta/2 \\
0 & \text{otherwise}
\end{cases}
\]  

(3.16)

In a finite volume method, the cell-averaged variables are defined at each cell as:

\[
\tilde{f} = \frac{1}{\Delta V} \int_{\Delta V} f(x) dx
\]  

(3.17)

Thus the cell average in the finite volume method, which will be implemented in the current study, belongs to the Top-hat filter. The Gaussian filter is also defined in physical space. The Gaussian filter function is the Gaussian distribution with zero mean and variance \( \sigma^2 = \Delta^2 / 12 \):

\[
G_f(x) = \frac{6}{\pi \Delta^2} \exp\left( -\frac{6}{\Delta^2} |x|^2 \right)
\]  

(3.18)

The Cutoff filter is a Top-hat filter in the spectral space:

\[
\hat{G}_f(k) = \begin{cases} 
1 & \text{if } |k| \leq \pi/\Delta \\
0 & \text{otherwise}
\end{cases}
\]  

(3.19)

A detailed description of properties of various filters can be found in textbook (Pope, 2002).

### 3.2.2 Filtered Governing Equations

Any instantaneous variable \( f \) can be defined as the sum of a Favre-averaged filtered scale \( \tilde{f} \) and a sub-grid scale \( f^* \)
\[ f = \bar{f} + f'' \tag{3.20} \]

where

\[ \bar{f} = \frac{\rho f}{\bar{\rho}} \tag{3.21} \]

Favre-averaging is used here to simplify the governing equations and to account for the variable density effects. However, \( \bar{\rho} f g \neq \bar{\rho} f g + \rho f' g' \) for filtering operations in LES, which is different from the Reynolds average (see Appendix A).

The filtered Favre-averaged Navier-Stokes equations for mass, momentum, energy and species concentration can be written as:

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} = 0
\]

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i \bar{u}_j + \bar{\rho} \delta_{ij})}{\partial x_j} = \frac{\partial (\bar{\tau}_{ij} - \bar{\tau}_{ij}^{\text{vis}})}{\partial x_j}
\]

\[
\frac{\partial \bar{\rho} \bar{E}}{\partial t} + \frac{\partial ((\bar{\rho} \bar{E} + \bar{p}) \bar{u}_i)}{\partial x_i} = \frac{\partial}{\partial x_i} (\bar{u}_i \bar{\tau}_{ij} + \lambda \frac{\partial \bar{\tau}}{\partial x_i} - H_{ij}^{\text{vis}} + \sigma_{ij}^{\text{vis}})
\]

\[
\frac{\partial \bar{\rho} \bar{Y}_k}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i \bar{Y}_k)}{\partial x_i} = \frac{\partial}{\partial x_j} (\bar{p} \bar{U}_{k,j} \bar{Y}_k - \Phi_{k,j}^{\text{vis}} - \Theta_{k,j}^{\text{vis}}) + \bar{\omega}_k
\]

The unclosed sub-grid terms are:
The SGS stresses term \( \tau_{ij}^{\text{sgs}} \), SGS energy fluxes term \( H_i^{\text{sgs}} \) and SGS species fluxes \( \Phi_{k,j}^{\text{sgs}} \) result from filtering these convective terms. The SGS viscous work term, \( \sigma_{ij}^{\text{sgs}} \), comes from correlations of the velocity field with the viscous stress tensor, and the SGS species diffusive fluxes term, \( \Theta_{k,j}^{\text{sgs}} \), comes from correlations of the velocity field with the species mass fractions with the diffusion velocities. The filtered species mass production rate, \( \bar{\omega}_k \), is also unclosed. The modeling of these SGS terms is discussed in detail in the following subsections.

In addition to the conservation equations, the equation of state must be filtered. Filtering the equation of state gives us:

\[
\bar{p} = \bar{p}_\infty T \sum_{k=1}^N \frac{\bar{Y}_k}{W_k} + \bar{p}_\infty \sum_{k=1}^N \frac{T_k^{\text{sgs}}}{W_k}
\]  

(3.31)

where \( T_k^{\text{sgs}} = \bar{\rho}T Y_k / \bar{p} - \bar{\rho} T \bar{Y}_k \). For low heat release, the correlation \( T_k^{\text{sgs}} \) can be expected to be negligible. However, this may be not true for high heat release cases. The difficulty and uncertainty in modeling this correlation means that it will be neglected without any justification in the current study (Calhoon and Menon, 1996).

The filtered total energy \( \bar{E} \) can be approximated as:
\[
\bar{E} = \bar{h} - \frac{\bar{p}}{\rho} + \frac{\tilde{u}_k^2}{2} + k^{\text{sgs}} = \bar{\psi} + \frac{\bar{P}}{\rho} C_p (T' d T') - \frac{\bar{p}}{\rho} + \frac{\tilde{u}_k^2}{2} + k^{\text{sgs}}
\]  
(3.32)

where \( \bar{\psi} = \sum_i Y_i h_{i,k}^{(0)} \) and \( k^{\text{sgs}} = \bar{\tau}_{kk}^{\text{sgs}} / 2 \bar{p} = \frac{1}{2} (\rho \bar{u}_k \bar{u}_k / \bar{p} - \tilde{u}_k^2) \).

### 3.2.3 Subgrid-Scale Models

The SGS modeling is the core of LES. Because small eddies dissipate most of the energy and are unresolved, SGS models are introduced to allow for the transfer of energy from larger to smaller scales and to mimic the drain of energy associated with the energy cascade. Most of the SGS models are based on an eddy-viscosity type model. In these models, the SGS stress \( \tau^{\text{sgs}} \) is related to the large-scale strain-rate tensor \( \bar{S}_{ij} \) as follows:

\[
\tau_{ij}^{\text{sgs}} - \frac{\delta_{ij}}{3} \tau_{kk}^{\text{sgs}} = -2 \nu_t \bar{S}_{ij}
\]
(3.33)

where \( \nu_t \) is the eddy viscosity and \( \bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_j}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial x_j} \right) \).

### 3.2.3.1 Algebraic Smagorinsky Type Model

In this kind of model, the eddy viscosity \( \nu_t \) is obtained algebraically to avoid solving additional equations. Usually the equilibrium hypothesis is made to simplify the problem and to obtain an algebraic model. The equilibrium hypothesis assumes that small-scale motions, which have shorter time scales than the large, energy-carrying eddies, can adjust more rapidly to perturbations and recover equilibrium nearly instantaneously. Under this assumption, a balance
exists between the SGS kinetic energy production term and the viscous dissipation term: \( \tau_{ij} \tilde{S}_{ij} = \varepsilon_v \). The Smagorinsky model based on the equilibrium hypothesis can be written as:

\[
\nu_t = (C_s \Delta)^2 |\tilde{S}| \tag{3.34}
\]

where \( \Delta \) is the filter width and \( |\tilde{S}| = (2 \tilde{S}_y \tilde{S}_y)^{1/2} \). The coefficient \( C_s \) can be determined from the isotropic turbulence decay or a prioric test. Erlebacher et al. (1992) extended the above model to include flow compressibility effects:

\[
\tau_{ij}^{\text{sgs}} = -2\nu_t \bar{p} (\tilde{S}_y - \frac{\tilde{S}_{kk} \delta_{ij}}{3}) + \frac{2}{3} \bar{p} k^{\text{sgs}} \delta_{ij} \tag{3.35}
\]

where \( \nu_t \) is the eddy viscosity.

\[
\nu_t = C_r (\Delta D)^2 |\tilde{S}| \tag{3.36}
\]

\[
k^{\text{sgs}} = C_r (\Delta D)^2 \tilde{S}_y \tilde{S}_{ij} \tag{3.37}
\]

where the dimensionless quantities \( C_r \) and \( C_t \) represent the compressible Smagorinsky constants.

The Van-Driest damping function \( D \) is used to take into account the inhomogeneities near the surface (Moin and Kim, 1982), and is expressed as

\[
D = 1 - \exp\left(1 - (y^+)^3 / 26^3\right) \tag{3.38}
\]

where \( y^+ = y u_c / \nu \) and \( u_c \) is friction velocity.

The subgrid energy fluxes term \( H_{ij}^{\text{sgs}} \) is modeled as:

\[
H_{ij}^{\text{sgs}} = -\bar{p} \nu_t \frac{\hat{h}}{\text{Pr}} \left( \frac{\partial \tilde{h}}{\partial x_j} + \tilde{u}_i \frac{\partial \tilde{u}_j}{\partial x_j} + \frac{1}{2} \frac{\partial k^{\text{sgs}}}{\partial x_j} \right) \tag{3.39}
\]
where $Pr_t$ represents the turbulent Prandtl number, a standard value 0.7 is used. The SGS viscous work term, $\sigma_{ij}^{\text{gs}}$, is neglected due to its small contribution to the total energy equation.

The convective species flux term is usually approximated as:

$$\Phi_{k,i}^{\text{sgs}} = -\overline{\nu_i} \frac{\partial \overline{Y_k}}{\partial x_i}$$

where $Sc_t$ is the turbulent Schmidt number. But the use of the gradient transport assumption for reactive species is questionable. The SGS species diffusive fluxes term, $\Theta_{k,j}^{\text{gs}}$, usually is also neglected.

The algebraic Smagorinsky type model described above is the most widely used model in LES. However, as pointed out by Moin et al. (1991), this model’s limitations are as follows. First, the optimal model constant must be changed for a different class of flows. The model does not have the correct limiting behavior near a wall. The SGS stress does not vanish in laminar flow and the model is found to be very dissipative in the laminar/transition region. The model does not account for the backscatter of energy from small to large scale, which has been shown to be of importance in the transition region.

### 3.2.3.2 Dynamic Smagorinsky Model

The dynamic model introduced by Germano et al. (1991) overcomes many of the aforementioned deficiencies in algebraic models. The dynamic model uses the assumption of scale invariance by applying the coefficient measured from the resolved scales to the SGS range. It calculates the model coefficients dynamically as a function of position from the information already contained in the resolved velocity field during the simulation (rather than treating it as an adjustable parameter as in the standard Smagorinsky model). The dynamic model uses resolved-
scale information at the grid-filter level and a coarser test-filter \( \hat{G}_j \) with characteristic \( \hat{\Lambda} > \Lambda \) (typically, \( \hat{\Lambda} = 2\Lambda \)) in order to compute the model parameters \( C_R \) and \( C_I \) as a function of space and time (Germano et al., 1991). Formally, the dynamical procedure is based on the Germano identity (Germano, 1992):

\[
L_{ij} = T_{ij} - < \tau_{ij}^{sgs} >
\]  

(3.41)

where \( L_{ij} = \langle \rho \hat{u}_i \hat{u}_j \rangle - \langle \rho \rangle \langle \hat{u}_i \hat{u}_j \rangle \) and \( T_{ij} = \langle \rho u_i u_j \rangle - \langle \rho \rangle \langle u_i u_j \rangle \). Here a Favre-filtered variable under a test-filter is defined as \( \hat{f} = \langle \rho f \rangle / \langle \rho \rangle \). The brackets \( < \cdot > \) denote the averaging operation based on the test filter. The following expressions can be derived for the dynamic evaluation of \( C_R \) and \( C_I \) using the least square minimization approach of Lilly (1992) for the momentum SGS stress tensor.

\[
C_R = \frac{< L_{ij} M_{ij} >}{< M_{kl} M_{kl} >} - \frac{1}{3} \frac{< L_{mn} M_{mn} >}{< M_{kl} M_{kl} >}
\]  

(3.42)

\[
C_I = \frac{< L_{kk} >}{< \beta - < \alpha > >}
\]  

(3.43)

The forms of \( M_{ij} \), \( \beta \) and \( \alpha \) are given as follows:

\[
M_{ij} = \beta_{ij} - < \alpha_{ij} >
\]  

(3.44)

\[
\beta_{ij} = -2\hat{\Lambda}^2 < \rho > | \vec{S} | ( \vec{S}_y - \frac{\delta_{ij}}{3} \vec{S}_k ) ; \quad \alpha_{ij} = -2\hat{\Lambda}^2 \bar{\rho} | \vec{S} | ( \vec{S}_y - \frac{\delta_{ij}}{3} \vec{S}_k )
\]  

(3.45)

\[
\beta = 2 < \rho > \hat{\Lambda}^2 | \vec{S} |^2 ; \quad \alpha = 2 \bar{\rho} \hat{\Lambda}^2 | \vec{S} |^2
\]  

(3.46)

The same idea for modeling the SGS turbulent stress can be employed to dynamically calculate the turbulent Prandtl number and Schmidt number in Eq. 3.39 and Eq. 3.40.
We implemented the algebraic Smagorinsky model in the current study although it may not be the best SGS model for the current work. There are two reasons: first, the best SGS model for swirling flows is still unknown; and second, the grid requirement for other models such as the dynamical model is normally stricter than the algebraic Smagorinsky model due to its double filters, both of which are required to be located in the inertial range.

3.3 Turbulent Combustion Models

Proper treatment of the filtered species mass production rate $\bar{\omega}_k$ comprises most of the difficulty in LES subgrid modeling because of the highly nonlinear behavior of the rate expression. The simplest method based on the Arrhenius law is to neglect the contribution from the subgrid scales as assuming perfect subgrid mixing. Some other combustion models, such as the level-set flamelet library approach, thickened-flame models, et al., (already reviewed in chapter 1), can also be used to complete the mathematical formulation. In this section, a detailed discussion is provided about the level-set flamelet library approach.

3.3.1 The Arrhenius Law Based on Filtered Quantities

The following relationship is used to express the net filtered production rate $\bar{\omega}_k$ of each species in a multi-step mechanism:

$$\bar{\omega}_k = W_0 \sum_{j=1}^{L} \left( \nu_{hj} - \nu_{li} \right) \left[ \tilde{k}_{hi} \prod_{k=1}^{N} \tilde{v}_{ik} \tilde{v}_{ik} \right], \quad k = 1, 2, ..., N$$  \hspace{1cm} (3.47)
where \( \tilde{X}_k \) represents the molar filtered concentration of species \( k \). \( \tilde{k}_{fi} \) and \( \tilde{k}_{bi} \) are the reaction rate constants of the forward and backward reactions, respectively, and takes the following form:

\[
\tilde{k}_i(\tilde{T}) = A_i \tilde{T}^b \exp(-E_i / R_m \tilde{T})
\]  (3.48)

where \( A, b, \) and \( E_i \) are empirical parameters and \( E_i \) represents the activation energy of reaction \( i \).

Modeling of the SGS reaction-rate term \( \tilde{\omega}_k \) using Eq. 3.48 often under-predicts the global turbulent rate (Charlette, 2002), because the unresolved flame is wrinkled at scales below the LES resolution, which typically increases the global reaction rate.

### 3.3.2 Regime Diagram in Premixed Turbulent Combustion

In a premixed combustion, the fuel and oxidizer are perfectly mixed before ignition. After the combustion process is initiated, if the unburned mixture lies within the flammability limits and the chemical reactions are very fast, a thin flame front develops and propagates upstream. The structure of a stationary, premixed, laminar flame is displayed in Fig. 3-1. Three characteristic layers can be defined: the preheat layer, the inner layer, and the oxidation layer (Peters, 2000). In the preheat layer, the unburned mixture enters the flame structure at the flame speed \( S_L \) and is preheated. In this layer, a balance exists between convection and diffusion. The second layer is a thin inner layer where the fuel is consumed. In this layer a diffusive-reactive balance exists and the chemical reactions primarily occur. The combustion process cannot be sustained if this layer is affected by turbulence because enhanced transport of heat and radicals out of the inner layer exceeds their production in the inner layer and extinguishes the flame. The last layer is the oxidation layer. In this layer, primarily oxidation reactions take place, though these reactions are of minor importance with respect to the flame characteristics. There are two
important length scales, the flame thickness $l_f$ and the inner layer thickness $l_\delta$, within the laminar flame structure. These two length scales can be related as $l_\delta = \delta l_f$. Peters (1991) shows that $\delta$ varies from $\delta = 0.1$ at atmospheric pressure to $\delta = 0.03$ at pressures around 30 atm.

![Diagram](image)

Fig. 3-1: Temperature and species-concentration distributions of laminar premixed flame of methane and air ($T_{in} = 660$ K, $\phi = 0.573$ and $p = 0.463$ MPa)

However, premixed turbulent combustion involves a wide range of length and time scales associated with chemical reactions and flow motions. Peters (2000) examined the problem of turbulence/chemistry interactions in terms of two non-dimensional parameters, turbulent Reynolds number $Re$ and turbulent Karlovitz number $Ka$, as defined below.

$$Re \approx \nu' / S_L / l_f$$  \hspace{1cm} (3.49)

$$Ka = t_f / t_\eta \approx l_f^2 / \eta^2$$  \hspace{1cm} (3.50)

where $\nu'$ is turbulent velocity fluctuation, $l$ is the turbulent integral length scale, $S_L$ and $l_f$ are the flame speed and thickness, respectively, $t_f$ and $t_\eta$ are the flame and the Kolmogorov time.
scales, respectively, and $\eta$ is the Kolmogorov length scale. Another Karlovitz number $Ka_\delta$, defined as the square of the ratio of the flame inner layer thickness $l_\delta$ to the Kolmogorov length scale $\eta$, is also introduced. Based on the relative magnitudes of these parameters, premixed turbulent combustion can be classified into four different regimes, as shown in Fig. 3-2. Corrugated flamelets occur when $Re > 1, v'/S_L > 1$ and $Ka < 1$. In this regime, the turbulent velocity fluctuation $v'$ is large enough to allow eddies to corrugate the flame front. The smallest eddies of size $\eta$, however, are still larger than the laminar flame thickness $l_F$, and thus cannot modify the flame structure. The interaction between eddies of all sizes and the laminar flame structure is purely kinematic. The chemical and transport processes within the flame remain essentially unchanged. A thin reaction zone exists when $Re > 1, v'/S_L > 1, Ka > 1$ and $Ka_\delta < 1$. In this regime, the smallest eddies of size $\eta$ are smaller than the laminar flame thickness $l_F$, and can penetrate into the bulk of the flame structure. They cannot enter into the inner layer, however, because the smallest eddies are larger than the thickness of the inner layer. Although the local transport of chemical species and energy are enhanced in the preheat zone, the chemical reactions that sustain the flame are essentially not influenced by turbulence since they do not penetrate the inner layer. The wrinkled flamelet regime ($Re > 1, v'/S_L < 1$ and $Ka < 1$) and the broken reaction zone ($Re > 1, v'/S_L > 1$, and $Ka_\delta > 1$) are two extreme situations with very weak turbulence intensities or with very small turbulence eddies which can alter the chemical reactions in the inner layer. These two regimes are usually not of practical interest for LPM gas turbine systems and will not be discussed here.
In both the thin reaction and corrugated-flamelet regimes, the inner layer of the laminar flame structure is not affected by turbulence. Therefore, based on the level-set flamelet approach, the premixed turbulent flame can be treated as a synthesis of thin reaction-diffusion layers, commonly referred to as flamelets (Herrmann, 2000), embedded in an otherwise inert turbulent flow field. When a Reynolds-average approach is used, the turbulent flame is viewed as the ensemble average of different laminar flamelets, which fluctuate randomly around the mean flame position in the normal direction under the effect of turbulence. For large-eddy simulations, the filter process is considered as a local volume average (Pope, 2000). The filtered mean flame also can be regarded as the average of different laminar flamelets, which randomly fluctuate around the mean flame position in the normal direction under the effects of unresolved small-scale turbulence. The mean location of flamelets is obtained by solving a level-set transport equation. After the structure of the laminar flamelet is determined by employing a finite rate chemistry model, a presumed PDF method can be used to determine the mean thermophysical properties such as species concentrations.

Fig. 3-2: Regime diagram of premixed turbulent combustion (after Peters, 2000)
3.3.2 Level-Set Flamelet Library Approach

3.3.2.1 Level-Set Equation for Laminar Premixed Flame

In level set methods, the location of the propagating premixed flame surface is defined by an iso-surface of a level set scalar \( G(x,t) = G_0 \). Then the iso-surface \( G_0 \) divides the flow field into an unburned part, \( G(x,t) < G_0 \), and a burned part, \( G(x,t) > G_0 \). Define the flame front equation as \( F(x,t) = G(x,t) - G_0 = 0 \), as shown in Fig. 3.3. At time \( t = t + dt \), a particle at \( F(x,t) = 0 \) moves to a new location \( x + dx = x + (u + S_L n) \cdot dt \), where \( n = -\nabla G / |\nabla G| \). Then we get:

\[
F(x + (u + S_L n) \cdot dt, t + dt) = 0 \tag{3.51}
\]

Using Taylor series, we obtain:

\[
0 = F(x,t) + (u + S_L n) \cdot dt \cdot \nabla F + dt \cdot \frac{\partial F}{\partial t} + O(dt^2) \tag{3.52}
\]

Let \( dt \to 0 \). The above equation becomes

\[
(u + S_L n) \cdot \nabla F + \frac{\partial F}{\partial t} = 0 \tag{3.53}
\]

Substitute \( F(x,t) = G(x,t) - G_0 \) into the above equation. A scalar-field \( G \) equation describing the evolution of a thin flame front can be written as follows:

\[
\frac{\partial \rho G}{\partial t} + \nabla \cdot \rho u G = \rho S_L |\nabla G| \tag{3.54}
\]
where the laminar flame speed $S_L$ for an idealized planar configuration depends on pressure, temperature, and mixture equivalence ratio (Williams, 1985). In reality, flame curvature and flow unsteadiness, which can be characterized by a stretch rate $\kappa$ (defined as the fractional rate of change of a flame surface area $\kappa = (d\delta A/dt)/\delta A$) have a significant impact on the flame speed $S_L$ (Clavin, 1985; Law and Sung, 2000). Depending on the Lewis number, the stretch rate can increase or decrease the flame speed. A linear model (Clavin, 1985) for a small stretch has been proposed to account for this effect.

$$S_L = S_L^0 - S_L^0 M \kappa$$

(3.55)

where $S_L^0$ is the laminar burning velocity of a plane, undisturbed premixed laminar flame, and $M$ the Markstein length, which is a function of mixture properties.
3.3.2.2 Level-Set Equation for Premixed Turbulent Flame

Upon filtering Eq. 3.54, the following Favre-averaged G-equation for LES is obtained

\[
\frac{\partial \bar{\rho} \bar{G}}{\partial t} + \nabla \cdot \bar{\rho} \bar{u} \bar{G} = -\nabla \cdot (\rho \bar{u} \bar{G} - \bar{\rho} \bar{u} \bar{G}) + \rho S_L \left| \nabla \bar{G} \right| \tag{3.56}
\]

The first term on the right-hand side of Eq. 3.56 is associated with turbulent transport. Since the original G equation is parabolic, this term cannot be approximated using a classical gradient-transport approach because of the reduction to an elliptic equation for \( \bar{G} \). According to Peters (2000), it could be modeled as:

\[
\nabla \cdot (\rho \bar{u} \bar{G} - \bar{\rho} \bar{u} \bar{G}) = \bar{\rho} D_t \bar{k} \left| \nabla \bar{G} \right| \tag{3.57}
\]

where \( D_t = v / \text{Pr} \) and \( \bar{k} \) is the filtered flame front curvature, \( \bar{k} = \nabla \cdot \bar{n} = \nabla \cdot (-\nabla \bar{G} / \left| \nabla \bar{G} \right|) \). The second term on the right-hand side of Eq. 3.56 represents turbulent flame propagation and can be related to the SGS turbulent flame speed \( S_T \) as follows:

\[
\bar{\rho} S_L \left| \nabla \bar{G} \right| = \bar{\rho} S_T \left| \nabla \bar{G} \right| \tag{3.58}
\]

Substitution of Eq. 3.57 and Eq. 3.58 into Eq. 3.56 leads to a modeled filtered G equation:

\[
\frac{\partial \bar{\rho} \bar{G}}{\partial t} + \nabla \cdot \bar{\rho} \bar{u} \bar{G} = \bar{\rho} S_T \left| \nabla \bar{G} \right| - \bar{\rho} D_t \bar{k} \left| \nabla \bar{G} \right| \tag{3.59}
\]

The SGS turbulent flame speed \( S_T \) needs to be treated. This closure generally takes the form (Lipatnikow and Chomiak, 2000):

\[
S_T = S_L \left( 1 + C \left( \frac{\bar{\nu}}{S_L} \right)^n \right) \tag{3.60}
\]
where $v'_\Delta$ is the SGS turbulent velocity fluctuation and may be modeled as

$$v'_\Delta = 2.0\lambda^3 (\nabla \times (\nabla^2 \vec{u})) \text{(Colin et al., 2000)}$$

The two constants $C$ and $n$ need be specified $(C \approx 2.0, n \approx 0.7)$ or dynamically determined (Im and Lund, 1997).

### 3.3.2.3 Presumed PDF Method

With the assumption that mean turbulent flame is an ensemble average or local volume average of different laminar flamelets that fluctuate randomly around the mean flame position in the normal direction under the effect of turbulence, the mean chemical composition of a premixed turbulent flame can be obtained using a presumed PDF method along with a resolved flamelet structure. To this end, the probability of finding the instantaneous flame front at a given position and instant needs be presumed. A reasonable choice appears to be a Gaussian distribution (Wirth et al, 1993; Plessing et al., 1999; Peter, 2000).

To demonstrate how to get the mean quantities of the turbulent flame, we first consider a one-dimensional steady turbulent flame propagating in the $x$ direction. We define $x$ as the location of the instantaneous flame front and $\tilde{x}$ as the location of the mean flame front. Then the turbulent flame thickness can be defined as $l_{F,t} = (\overline{(x-\tilde{x})^2})^{1/2}$, which is the variance of the flame location. With the assumption of a Gaussian distribution, the probability of finding a flame front at $x$ can be written as:

$$P(x) = \frac{1}{(2\pi l_{F,t}^2)^{1/2}} \exp\left(-\frac{(x-\tilde{x})^2}{2l_{F,t}^2}\right)$$

(3.61)

where $\tilde{x} = \int_{-\infty}^{\infty} xP(x)dx$; $l_{F,t}^2 = (\overline{(x-\tilde{x})^2}) = \int_{-\infty}^{\infty} (x-\tilde{x})^2 P(x)dx$
We first assume that the structure of the laminar flamelet was resolved as $Y_n = Y_n(x_n)$, where $x_n$ is the normal distance to the center of the inner layer (defined as the flame front). In a realization, there is an instantaneous flamelet at location $x$; the instantaneous mass fraction of species at another location $x_A$ is recorded as: $Y_i(x_A) = Y_n(x_n) = Y_n(x_A - x)$. The mean quantities at location $x_A$ are:

$$\tilde{Y}_i(x_A) = \int_{-\infty}^{\infty} Y_n(x_A - x)P(x)dx$$  \hspace{1cm} \text{(3.62)}$$

since $x_n = x_A - x$:

$$\tilde{Y}_i(x_A) = \int_{-\infty}^{\infty} Y_n(x_n)P(x_A - x_n)dx_n = \int_{-\infty}^{\infty} Y_n(x_n)P_n(x_n)dx_n$$  \hspace{1cm} \text{(3.63)}$$

where

$$P_n(x_n) = P(x_A - x_n) = \frac{1}{(2\pi l_{F,i}^2)^{1/2}} \exp\left(-\frac{(x_n - (x_A - \bar{x}))^2}{2l_{F,i}^2}\right)$$  \hspace{1cm} \text{(3.64)}$$

$$l_{F,i}^2 = (x - \bar{x})^2 = (x_n - (x_A - \bar{x}))^2 = \int_{-\infty}^{\infty} (x_n - (x_A - \bar{x}))^2 P(x_n)dx_n$$  \hspace{1cm} \text{(3.65)}$$

The above analysis indicates that the mean composition at any location $x_A$ is determined by the resolved laminar profile $Y_n(x_n)$ and the Gaussian PDF with mean value $x_A - \bar{x}$ (which is the distance of location $x_A$ to the mean flame front $\bar{x}$) and variance $l_{F,i}^2$ over the normal direction. Note that $l_{F,i}$ is defined at the location of the flame front.

As mentioned before, the filtered $G$ equation is valid only for the flame front, but not the entire flow-field. Thus we can define $\tilde{G}(x,t)$ as a distance function normal to the flame surface
outside the flame front using a re-initialization process $|\nabla \tilde{G}| = 1$. The SGS turbulent flame thickness $l_{F,\tau}$, which measures the flame front fluctuations in the normal direction, can be defined as:

$$l_{F,\tau} = (\bar{G} - \tilde{G}_0)^2 = (\bar{G}^\prime)^{1/2}_{\tilde{G} = \tilde{G}_0}$$  \hspace{1cm} (3.66)

where $(\bar{G}^\prime)^{1/2}_{\tilde{G} = \tilde{G}_0}$ is a conditional variance evaluated at the flame front $\tilde{G} = \tilde{G}_0$. Again, note that the flame thickness can only be defined at the flame surface. Then a Gaussian-shape of PDF can be obtained:

$$P(G; x, t) = \frac{1}{\sqrt{2\pi (\bar{G}_0^\prime)^{1/2}_0}} \exp\left\{ -\frac{[G - \tilde{G}(x, t)]^2}{2(\bar{G}^\prime)_0^2} \right\}$$  \hspace{1cm} (3.67)

Here in the present study, the effects of strain on the flame structure and orientation between the instantaneous and mean flame surfaces are not included.

The averaged mass fraction of species $i$ can be calculated by:

$$\bar{Y}_i(x, t) = \int_{-\infty}^{\infty} Y_i(G, t)P(G, x, t)dG$$  \hspace{1cm} (3.68)

However, in order to obtain a presumed PDF, information about the flame thickness or the G variance is needed. The filtered flame thickness $l_{F,\tau}$ is determined by the fluctuation of laminar flamelets under the effect of unresolved small-scale turbulence. A transport equation for the filtered G variance can be derived (see Appendix B).

$$\frac{\partial \bar{\rho \tilde{G}}^\prime}{\partial t} + \nabla \cdot (\bar{\rho \tilde{u}} \bar{G}^\prime) = -\nabla \cdot (\bar{\rho \tilde{u}} \bar{G}^\prime) - \bar{\rho \tilde{u}} \bar{G}^\prime - 2\bar{\rho} \bar{G}^\prime \nabla \tilde{G}$$
$$+ 2\bar{G}^\prime \bar{\rho} \nabla \cdot (\bar{\rho \tilde{u}} \tilde{G} - \bar{\rho \tilde{u}} \tilde{G}) + 2\bar{\rho} S \bar{G}^\prime \sigma$$  \hspace{1cm} (3.69)
where $\sigma = |\nabla G|$. But such a model has not yet been developed within the context of LES. A simple approach based on dimensional analysis is thus implemented here. The SGS flame thickness $l_{F,s}$ is a function of the laminar flame thickness $l_F$, filter width $\Delta$, SGS turbulent velocity fluctuation $v'_{\Delta}$ and other parameters.

$$l_{F,s} = f(l_F, \Delta, v'_{\Delta}, \ldots) \quad (3.70)$$

In the limits of an infinitely thin flame, the SGS flame thickness $l_{F,s}$ will become independent of laminar flame thickness $l_F$:

$$l_{F,s} = f(\Delta, v'_{\Delta}, \ldots) \quad (3.71)$$

Peters (2000) proposed a simple model in the context of RANS, $l_{F,s} \approx C \cdot l$, where $l$ is the integral length scale and $C$ is a constant. A similar approach is taken for LES, accordingly.

$$l_{F,s} = C_0 \Delta + l_F \quad (3.72)$$

where $C_0 (\approx 1)$ is an empirical constant. The model suffers from a major limitation that the effects of small-scale motions on flame thickness are totally represented by the filter width, a situation rather remote from reality. A transport equation for the $G$ variance is required in order to correctly address this problem.

### 3.3.2.4 Generation of the Laminar Flamelet Library

With the assumption that a turbulent premixed flame is a collection of flamelets embedded in an otherwise inert turbulent flow field, the inner structure of a premixed flame can thus be
calculated separately from the turbulent flow calculation, taking into account finite-rate chemistry and elementary reaction mechanisms. There are several ways to generate a laminar flamelet library. The simplest approach is to assume infinitely fast chemistry and a quasi-laminar flame without an inner structure. All of the flow quantities change abruptly from the unburned to the burned state. Unfortunately, this neglects the effects of finite rate chemistry and transport phenomena inherent in a flame.

Another way to determine the inner structure of a flame is to solve a flamelet equation (Peter, 2000), valid for both the corrugated-flamelet and the thin-reaction regions in the regime diagram for premixed turbulent combustion. This approach is not used because of its complexity. In the present study, a flamelet library is established by solving a system of transport equations for the temperature and species-concentration fields for a freely propagation plane flame. The entire flame is assumed to be laminar without the influence of turbulence. This method, originally proposed by Nilsson and Bai (2001), is adopted here because of its ease of implementation.

### 3.3.2.5 Re-Initialization Process

The $\widetilde{G}$ variable is defined as a distance function outside the flame front, but this property is not conserved by the level-set equation. It needs to be enforced by a re-initialization process. From the numerical point of view, because the discretization of the level-set equation contains the spatial gradients of $\widetilde{G}$, a dependency on values of $\widetilde{G} \neq \widetilde{G}_0$ near the flame surface is introduced. It is important to keep the values of the gradient of $\widetilde{G}$ near unity in order not to undermine the numerical accuracy (Herrmann, 2000). Several methods have been proposed to enforce the
condition \(|\nabla \tilde{G}| = 1\) and render the level-set function a signed distance (with negative distance on one side and positive distance on the other side). The method developed by Sussman et al. (1994) and Russo et al. (2000) with a narrow banding strategy (1999) is used here, by solving the following equations iteratively to a steady state.

\[
\begin{align*}
\frac{\partial \tilde{G}}{\partial \tau} &= \text{sgn}(\tilde{G}_0)(1 - |\nabla \tilde{G}|) \\
\tilde{G}(x, 0) &= \tilde{G}_0(x)
\end{align*}
\] (3.73)

where \(\text{sgn}(\tilde{G}_0)\) is a sign function, defined as:

\[
\text{sgn}(x) = \begin{cases} 
1 & \text{if } x > 0 \\
0 & \text{if } x = 0 \\
-1 & \text{if } x < 0
\end{cases}
\] (3.74)

The steady solution satisfies the condition of \(|\nabla \tilde{G}| = 1\) and has the same zero-level as \(\tilde{G}_0\). Thus the desired signed distance function is obtained.

The coupling of the flow equations and the flamelet library is treated following the approach used by Herrmann (2000). The thermophysical variables extracted from the flamelet library are the ratio of specific heats \(\gamma\), the gas constant \(R\) and the enthalpy of formation of the mixture \(\psi = \sum_{k=1}^{N} Y_k \Delta h^R_{y,k}\). The temperature is determined through Eq. 3.32 using the preceding three variables and other flow properties obtained from the flow equations. Heat release is also obtained from the flamelet library.
4.1 Mathematical Equations

The three-dimensional, unsteady, density-weighted, filtered forms of the compressible Navier-Stokes equations (without body forces) and level-set equation can be expressed as:

\[
\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial (\mathbf{E} - \mathbf{E}_v)}{\partial x} + \frac{\partial (\mathbf{F} - \mathbf{F}_v)}{\partial y} + \frac{\partial (\mathbf{G} - \mathbf{G}_v)}{\partial z} = \mathbf{H}
\]  

(4.1)

where the vectors \(\mathbf{Q}, \mathbf{E}, \mathbf{F}, \mathbf{G}, \mathbf{E}_v, \mathbf{F}_v, \mathbf{G}_v,\) and \(\mathbf{H}\) are defined as:

\[
\mathbf{Q} = \left( \rho, \rho \bar{u}, \rho \bar{v}, \rho \bar{w}, \rho \bar{E}, \rho \bar{G} \right)^T
\]

(4.2)

\[
\mathbf{E} = \left( \rho \bar{u}, \rho \bar{u}^2 + \bar{p}, \rho \bar{u} \bar{v}, \rho \bar{u} \bar{w}, \left( \rho \bar{E} + \bar{p} \right) \bar{u}, \rho \bar{u} \bar{G} \right)^T
\]

(4.3)

\[
\mathbf{F} = \left( \rho \bar{v}, \rho \bar{u} \bar{v}, \rho \bar{v}^2 + \bar{p}, \rho \bar{v} \bar{w}, \left( \rho \bar{E} + \bar{p} \right) \bar{v}, \rho \bar{v} \bar{G} \right)^T
\]

(4.4)

\[
\mathbf{G} = \left( \rho \bar{w}, \rho \bar{u} \bar{w}, \rho \bar{v} \bar{w}, \rho \bar{w}^2 + \bar{p}, \left( \rho \bar{E} + \bar{p} \right) \bar{w}, \rho \bar{w} \bar{G} \right)^T
\]

(4.5)

\[
\mathbf{E}_v = \left( 0, \bar{r}_{xx} - \tau_{sgx}, \bar{r}_{xy} - \tau_{sgx}, \bar{r}_{xz} - \tau_{sgx}, \bar{u} \bar{r}_{xx} + v \bar{r}_{xy} + w \bar{r}_{xz} + \bar{G}_x - H_{sgx} + \sigma_{sgx}, 0 \right)^T
\]

(4.6)

\[
\mathbf{F}_v = \left( 0, \bar{r}_{xy} - \tau_{sgx}, \bar{r}_{yy} - \tau_{sgy}, \bar{r}_{yz} - \tau_{sgy}, \bar{u} \bar{r}_{xy} + v \bar{r}_{yy} + w \bar{r}_{yz} + \bar{G}_y - H_{sgy} + \sigma_{sgy}, 0 \right)^T
\]

(4.7)

\[
\mathbf{G}_v = \left( 0, \bar{r}_{xz} - \tau_{sgx}, \bar{r}_{yz} - \tau_{sgy}, \bar{r}_{zz} - \tau_{sgz}, \bar{u} \bar{r}_{xz} + v \bar{r}_{yz} + w \bar{r}_{zz} + \bar{G}_z - H_{sgz} + \sigma_{sgz}, 0 \right)^T
\]

(4.8)

\[
\mathbf{H} = \left( 0, 0, 0, 0, \rho \bar{S}_T \left| \nabla \bar{G} \right| - \rho \bar{D} \bar{k} \left| \nabla \bar{G} \right| \right)^T
\]

(4.9)
Each nomenclature is defined beforehand and the superscript $T$ stands for the transpose of the vector.

4.2 Spatial Discretization: Finite Volume Approach

4.2.1 Finite Volume Approach

The governing equations are solved numerically by means of a finite-volume approach. This method allows for the treatment of arbitrary geometry. To utilize the finite-volume approach, the governing equation is integrated over the control volume $V$ enclosed by the surface $S$ in the physical domain as:

$$\iiint \left( \frac{\partial Q}{\partial t} + \frac{\partial (E - E_x)}{\partial x} + \frac{\partial (F - F_y)}{\partial y} + \frac{\partial (G - G_z)}{\partial z} - H \right) dV = 0 \quad (4.10)$$
Using the Gauss divergence theorem, the integral conservation equation takes the following form for the three-dimensional cell with six surfaces, as shown in Fig. 4-1:

\[
\iiint \frac{\partial \mathbf{Q}}{\partial t} dV + \oint_{S_\xi} \mathbf{W} \cdot \mathbf{n}_\xi dS_\xi + \oint_{S_\eta} \mathbf{W} \cdot \mathbf{n}_\eta dS_\eta + \oint_{S_\zeta} \mathbf{W} \cdot \mathbf{n}_\zeta dS_\zeta = \iiint \mathbf{H} dV \tag{4.11}
\]

where

\[
\mathbf{W} = (\mathbf{E} - \mathbf{E}_v)\mathbf{i} + (\mathbf{F} - \mathbf{F}_v)\mathbf{j} + (\mathbf{G} - \mathbf{G}_v)\mathbf{k} \tag{4.12}
\]

and \(\mathbf{n}_\xi\), \(\mathbf{n}_\eta\), and \(\mathbf{n}_\zeta\) are unit normal vectors to the surface in the \(\xi\), \(\eta\), and \(\zeta\)-directions, respectively. The unit normal vectors are related to cell surface area \(S_\xi\), \(S_\eta\), and \(S_\zeta\) as:

\[
\mathbf{n}_\xi = \frac{\left( S_{\xi x} \mathbf{i} + S_{\xi y} \mathbf{j} + S_{\xi z} \mathbf{k} \right)}{|S_\xi|}
\]

\[
\mathbf{n}_\eta = \frac{\left( S_{\eta x} \mathbf{i} + S_{\eta y} \mathbf{j} + S_{\eta z} \mathbf{k} \right)}{|S_\eta|}
\]

\[
\mathbf{n}_\zeta = \frac{\left( S_{\zeta x} \mathbf{i} + S_{\zeta y} \mathbf{j} + S_{\zeta z} \mathbf{k} \right)}{|S_\zeta|}
\]

The cell surface areas are defined as:

\[
S_\xi = \frac{1}{2} \mathbf{r}_{72} \times \mathbf{r}_{36} = \frac{1}{2} \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x_2 - x_7 & y_2 - y_7 & z_2 - z_7 \\ x_6 - x_3 & y_6 - y_3 & z_6 - z_3 \end{vmatrix} = S_{\xi x}\mathbf{i} + S_{\xi y}\mathbf{j} + S_{\xi z}\mathbf{k}
\]

\[
S_\eta = \frac{1}{2} \mathbf{r}_{86} \times \mathbf{r}_{75} = \frac{1}{2} \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x_6 - x_8 & y_6 - y_8 & z_6 - z_8 \\ x_5 - x_7 & y_5 - y_7 & z_5 - z_7 \end{vmatrix} = S_{\eta x}\mathbf{i} + S_{\eta y}\mathbf{j} + S_{\eta z}\mathbf{k}
\]

\[
S_\zeta = \frac{1}{2} \mathbf{r}_{74} \times \mathbf{r}_{83} = \frac{1}{2} \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x_4 - x_7 & y_4 - y_7 & z_4 - z_7 \\ x_3 - x_8 & y_3 - y_8 & z_3 - z_8 \end{vmatrix} = S_{\zeta x}\mathbf{i} + S_{\zeta y}\mathbf{j} + S_{\zeta z}\mathbf{k}
\]
The magnitude of each surface vector can be obtained by
\[ \left| \vec{\mathbf{S}}_\xi \right| = \left( S_{\xi x}^2 + S_{\xi y}^2 + S_{\xi z}^2 \right)^{1/2} \]
\[ \left| \vec{\mathbf{S}}_\eta \right| = \left( S_{\eta x}^2 + S_{\eta y}^2 + S_{\eta z}^2 \right)^{1/2} \] \hfill (4.15)
\[ \left| \vec{\mathbf{S}}_\zeta \right| = \left( S_{\zeta x}^2 + S_{\zeta y}^2 + S_{\zeta z}^2 \right)^{1/2} \]

The cell volume \( \Delta V \) associated with each cell can be evaluated using Kordulla and Vinokur’s (1983) formula:
\[ \Delta V = \frac{1}{2} r_{12} \left( \vec{\mathbf{S}}_\xi + \vec{\mathbf{S}}_\eta + \vec{\mathbf{S}}_\zeta \right) \] \hfill (4.16)

We also define cell surface areas per cell volume as:
\[ \tilde{\mathbf{S}}_\xi = \mathbf{S}_\xi / \Delta V, \quad \tilde{\mathbf{S}}_\eta = \mathbf{S}_\eta / \Delta V, \quad \tilde{\mathbf{S}}_\zeta = \mathbf{S}_\zeta / \Delta V \]

Assuming the increments \( \Delta \xi = \Delta \eta = \Delta \zeta = 1 \) in the body-fitted coordinate system and substituting Eq. 4.12 and Eq. 4.13 into Eq. 4.11 yields the following governing equation in the general coordinates:
\[ \frac{\Delta \mathbf{Q}}{\Delta t} + \left( \mathbf{E}_\xi - \mathbf{E}_\phi \right)_{i-1/2,j,k}^{i+1/2,j,k} + \left( \mathbf{F}_\eta - \mathbf{F}_\phi \right)_{i,j-1/2,k}^{i,j+1/2,k} + \left( \mathbf{G}_\zeta - \mathbf{G}_\phi \right)_{i,j,k-1/2}^{i,j,k+1/2} = \mathbf{H} \] \hfill (4.17)

where the vectors \( \mathbf{E}_\xi, \mathbf{F}_\eta, \mathbf{G}_\zeta, \mathbf{E}_\phi, \mathbf{F}_\phi, \mathbf{G}_\phi \), and \( \Delta \mathbf{Q} \) are defined as:
\[ \Delta \mathbf{Q} = \mathbf{Q}^{n+1} - \mathbf{Q}^n \]
\[ \mathbf{E}_\xi = \left( \tilde{\mathbf{S}}_{\xi x} E + \tilde{\mathbf{S}}_{\xi y} F + \tilde{\mathbf{S}}_{\xi z} G \right) \quad \mathbf{E}_\phi = \left( \tilde{\mathbf{S}}_{\phi x} E + \tilde{\mathbf{S}}_{\phi y} F + \tilde{\mathbf{S}}_{\phi z} G \right) \]
\[ \mathbf{F}_\eta = \left( \tilde{\mathbf{S}}_{\eta x} E + \tilde{\mathbf{S}}_{\eta y} F + \tilde{\mathbf{S}}_{\eta z} G \right) \quad \mathbf{F}_\phi = \left( \tilde{\mathbf{S}}_{\phi x} E + \tilde{\mathbf{S}}_{\phi y} F + \tilde{\mathbf{S}}_{\phi z} G \right) \]
\[ \mathbf{G}_\zeta = \left( \tilde{\mathbf{S}}_{\zeta x} E + \tilde{\mathbf{S}}_{\zeta y} F + \tilde{\mathbf{S}}_{\zeta z} G \right) \quad \mathbf{G}_\phi = \left( \tilde{\mathbf{S}}_{\phi x} E + \tilde{\mathbf{S}}_{\phi y} F + \tilde{\mathbf{S}}_{\phi z} G \right) \] \hfill (4.18)
The quantities \( E_{\xi,j+1/2,j,k}, E_{\eta,j+1/2,j,k}, E_{\zeta,j+1/2,j,k}, F_{\eta,j+1/2,j,k}, F_{\eta,j+1/2,j,k}, G_{\xi,j+1/2,j,k} \) and \( G_{\eta,j+1/2,j,k} \) represent the numerical fluxes associated with each cell interface (see Fig. 4-1). \( \tilde{S} \) represents cell surface areas per cell volume. In fact, the above analysis describes the transformation of a quadrilateral cell with a volume \( \Delta V \) in \( x-y-z \) coordinates to a cubic cell with unit volume in the general coordinate (i.e., \( \xi-\eta-\zeta \) coordinates).

The maximum time increment \( \Delta t \) of each cell can be evaluated by:

\[
\Delta t = \frac{\Delta t_{\xi} \Delta t_{\eta} \Delta t_{\zeta}}{\Delta t_{\xi} + \Delta t_{\eta} + \Delta t_{\zeta}}
\]  

(4.19)

where

\[
\Delta t_{\xi} = \frac{CFL \cdot \Delta V}{|\bar{u}S_{\xi} + \bar{v}S_{\eta} + \bar{w}S_{\zeta}| + c|\bar{S}_{\xi}|};
\]

\[
\Delta t_{\eta} = \frac{CFL \cdot \Delta V}{|\bar{u}S_{\eta} + \bar{v}S_{\eta} + \bar{w}S_{\zeta}| + c|\bar{S}_{\eta}|};
\]

\[
\Delta t_{\zeta} = \frac{CFL \cdot \Delta V}{|\bar{u}S_{\zeta} + \bar{v}S_{\xi} + \bar{w}S_{\zeta}| + c|\bar{S}_{\zeta}|};
\]

and \( c = \sqrt{\gamma RT} \) is the local speed of sound.

### 4.2.2 Evaluation of Inviscid Fluxes

Different approaches used in evaluating the numerical fluxes lead to different schemes with disparate numerical characteristics. For the central difference scheme, the convective flux at any cell face in the \( \xi \)-direction can be written as:

\[
\hat{E}_{\xi,j+1/2,j} = \frac{1}{2} \left[ E_{\xi}(Q^L) + E_{\xi}(Q^R) \right]
\]

(4.20)
where the left and right stencils are used to give the desired accuracy. The above equation corresponds to the stencil illustrated in Fig. 4-2. The superscripts $L$ and $R$ represent the left and right cells. Depending on the manner in which these terms are evaluated, a wide variety of central and upwind schemes can be obtained. In the present work, the methodology proposed by Rai and Chakravarthy (1993) is used. Accordingly the numerical flux in Eq. 4.17 is computed as:

$$
\hat{E}_{\xi,j+1/2,j,k} = \hat{E}_{\xi,j+1/2,j,k} - \phi^{(4)}_{i+1/2,j,k} \left( \frac{\hat{E}_{\xi,j+3/2,j,k} - 2\hat{E}_{\xi,j+1/2,j,k} + \hat{E}_{\xi,j+1/2,j,k}}{24} \right) \quad (4.21)
$$

where $\phi^{(4)}$ is the flux limiter. This term switches the truncation error associated with the flux-difference from fourth-order accuracy when $\phi^{(4)} = 1$, to second-order accuracy when $\phi^{(4)} = 0$. To evaluate Eq. 4.20 regarding the desired accuracy, the left and right state terms in Eq. 4.21 must be computed using the same or higher order accuracy. These terms are written as follows to facilitate easy switching and make the scheme TVD (total variation diminishing).

Fig. 4-2: Schematic diagram of the stencil used in evaluating inviscid flux terms in the $x - y$ plane
These stencils can be used to get fifth-order accuracy \( \phi(4) = 1, \phi(2) = 1 \), third-order accuracy \( \phi(4) = 0, \phi(2) = 1 \), and first-order accuracy \( \phi(4) = 0, \phi(2) = 0 \), respectively. The present work utilizes second-order overall accuracy for spatial discretization with the exception of close to the physical boundaries. The third-order accurate evaluation of the left and right states is thus employed. The fluxes in \( \eta \), and \( \zeta \)-directions can be computed in a similar fashion as above.

\[
\begin{align*}
Q^L_{i+1/2,j,k} &= Q_{i,j,k} + \phi_{i+1/2,j,k}^{(2)} \left( \frac{3\nabla Q_{i+1,j,k} + \nabla Q_{i,j,k}}{8} \right) \\
&\quad + \phi_{i+1/2,j,k}^{(4)} \left( \frac{-5\nabla Q_{i+2,j,k} + 7\nabla Q_{i+1,j,k} + \nabla Q_{i,j,k} - 3\nabla Q_{i-1,j,k}}{128} \right) \\
Q^R_{i+1/2,j,k} &= Q_{i,j,k} - \phi_{i+1/2,j,k}^{(2)} \left( \frac{\nabla Q_{i+2,j,k} + 3\nabla Q_{i+1,j,k}}{8} \right) \\
&\quad + \phi_{i+1/2,j,k}^{(4)} \left( \frac{3\nabla Q_{i+3,j,k} - \nabla Q_{i+2,j,k} - 7\nabla Q_{i+1,j,k} + 5\nabla Q_{i,j,k}}{128} \right) \\
\n\nabla Q_{i,j} &= Q_{i,j} - Q_{i-1,j} \\
\end{align*}
\]

\( Q_{i,j,k} \) is the flux at the center of the control volume. The fluxes in \( \eta \) and \( \zeta \)-directions can be computed in a similar fashion as above.

### 4.2.3 Evaluation of Viscous and SGS Fluxes

A three-dimensional auxiliary cell is shown schematically by the dash-dotted lines in Fig. 4-3. The viscous fluxes need to be evaluated at the center of the cell faces, i.e., \( i+1/2, j, k \) for the viscous flux in the axial direction. Using the Gauss divergence theorem and applying it to a small control volume \( \Delta V \), the viscous fluxes can be approximated as:

\[
\nabla \cdot \vec{f} = \frac{1}{\Delta V} \int_{S} \vec{f} \cdot \vec{n} dS \\
\]

\( \vec{f} \) is the viscous flux vector, and \( \vec{n} \) is the outward normal vector at the control volume boundary.
Applying the above formulation to the auxiliary cell at \((i+1/2, j, k)\) gives:

\[
\left( \frac{\partial f}{\partial x} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\varphi_x} \bigg|_{i+1/2,j,k} - f S_{\varphi_x} \bigg|_{i,j,k} + f S_{\varphi_x} \bigg|_{i+1, j+1/2, k} - f S_{\varphi_x} \bigg|_{i+1/2,j,k+1/2} \right]
\]

Similarly,

\[
\left( \frac{\partial f}{\partial y} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\varphi_y} \bigg|_{i+1/2,j,k} - f S_{\varphi_y} \bigg|_{i,j,k} + f S_{\varphi_y} \bigg|_{i+1, j+1/2, k} - f S_{\varphi_y} \bigg|_{i+1/2,j,k+1/2} \right]
\]

\[
\left( \frac{\partial f}{\partial z} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\varphi_z} \bigg|_{i+1/2,j,k} - f S_{\varphi_z} \bigg|_{i,j,k} + f S_{\varphi_z} \bigg|_{i+1, j+1/2, k} - f S_{\varphi_z} \bigg|_{i+1/2,j,k+1/2} \right]
\]

**Fig. 4-3:** Schematic diagram for a three-dimensional auxiliary cell
Note that $f$ in the above equations are elements of the viscous flux vectors $E_{q_j}, F_{p_j}$ or $G_{q_j}$.

Physical variables with one-half indices need to be interpolated from the quantities at the neighboring cell centers and are given as,

$$f_{i+1/2,j+1/2,k} = \frac{1}{4}(f_{i,j,k} + f_{i+1,j,k} + f_{i+1,j+1,k} + f_{i,j+1,k})$$  \hspace{1cm} (4.29)

$$f_{i+1/2,j,k+1/2} = \frac{1}{4}(f_{i,j,k} + f_{i+1,j,k} + f_{i+1,j+1,k} + f_{i,j+1,k})$$

The evaluation of SGS fluxes follows a similar procedure as for the viscous and diffusive fluxes.

4.2.4 Evaluation of Artificial Dissipation

Artificial dissipation plays a crucial role in the stability of a numerical scheme based on central differencing. The form of these artificial dissipation terms depends on the order of accuracy of the numerical scheme, and must be higher-order accurate to keep its magnitude minimal. For the present case, the numerical differentiation of the flux vectors is second-order accurate in the core region of the computational domain. Accordingly, the artificial dissipation is fourth-order accurate. The order of accuracy of the numerical scheme decreases near the physical boundary, and the artificial dissipation also goes to a lower order. The form of numerical dissipation used in the present schemes is quite often a blending of second- and fourth-order dissipation terms. The second-order terms are used to prevent oscillations near shock waves and in flame zones to prevent spurious oscillations within such thin regions, while the fourth-order terms are important for stability and convergence. The standard dissipation model can be written as:

$$\mathbf{AD} = \text{artificial dissipation}$$

$$= d_{i+1/2,j,k} - d_{i-1/2,j,k}$$  \hspace{1cm} (4.30)
where

\[ d_{i+1/2,j,k}^{(2)} = \sum_{i} \frac{1}{8} \frac{\partial Q}{\partial \xi_{i+1/2,j,k}} - \frac{1}{8} \frac{\partial^3 Q}{\partial \xi_{i+1/2,j,k}^3} + \frac{1}{8} \frac{\partial^5 Q}{\partial \xi_{i+1/2,j,k}^5} \]

(4.31)

where \( \epsilon_2, \epsilon_4, \epsilon_6 \) correspond to the coefficients of the second-, fourth- and sixth-order accurate artificial dissipation terms and in the present formulation, \( \Delta \xi = 1 \).

Even though the standard dissipation model has been proven to be reasonably effective in many cases, there are strong motivations for reducing the numerical dissipation being produced. Also, the standard model has difficulties in hypersonic flow and reactive flow with steep discontinuities near the flame front as in the present case. A matrix dissipation model was constructed by Swanson and Turkel (1992) and by Jorgenson and Turkel (1993) to overcome the above difficulties. In their model,

\[ d_{i+1/2,j,k}^{(2)} = \epsilon_{i+1/2,j,k}^{(2)} \left| \hat{A}_{i+1/2,j,k} \right| \frac{\partial Q}{\partial \xi_{i+1/2,j,k}} - \epsilon_{i+1/2,j,k}^{(4)} \left| \hat{A}_{i+1/2,j,k} \right| \frac{\partial^3 Q}{\partial \xi_{i+1/2,j,k}^3} \]

(4.32)

with

\[ \left| \hat{A} \right| = M_{\xi} \left| \hat{A}_{\xi} \right| M^{-1}_{\xi} \]

(4.33)

\[ \epsilon_{i+1/2,j,k}^{(2)} = \kappa_{i+1/2,j,k}^{(2)} \max (v_{i-1,j,k}, v_{i,j,k}^+, v_{i-1,j,k}^+, v_{i+1,j,k}^+) \]

(4.34)

\[ v_{i,j,k} = \frac{|p_{i,j,k} - 2p_{i+1,j,k}|}{p_{i-1,j,k} + 2p_{i,j,k} + p_{i+1,j,k}} \]

(4.35)

\[ \epsilon_{i+1/2,j,k}^{(4)} = \max (0, (\kappa^{(4)} - \epsilon_{i+1/2,j,k}^{(2)})) \]

(4.36)

\[ \kappa^{(2)} = \frac{1}{4} - \frac{1}{2}, \quad \kappa^{(4)} = \frac{1}{64} - \frac{1}{32} \]

(4.37)
The matrix dissipation model causes the central-difference scheme to closely resemble an upwind scheme near flow discontinuities and have the total variation diminishing (TVD) property, which prevents the occurrence of spurious oscillations. The terms \( \mathbf{M}_\xi \) and \( \mathbf{M}_\xi^{-1} \) are the right and left eigenvectors matrices, which diagonalize \( \mathbf{A} \), where \( \mathbf{A} = \frac{\partial \mathbf{E}_\xi}{\partial \mathbf{Q}} \). The eigenvalues of the flux Jacobin matrix \( \mathbf{A} \) are:

\[
\begin{align*}
\lambda_1 &= \lambda_2 = \lambda_3 = \lambda_6 = U \\
\lambda_{4,5} &= U \pm C
\end{align*}
\]  

(4.38)

where \( U = \tilde{S}_\xi u + \tilde{S}_\xi v + \tilde{S}_\xi w \) and \( C = c \tilde{S}_\xi \). The term \( \hat{\Lambda}_\xi \) in Eq. 4.34 represents the modified diagonal matrix of eigenvalues \( \hat{\Lambda}_\xi = \text{diag}(\hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3, \hat{\lambda}_4, \hat{\lambda}_5, \hat{\lambda}_6) \) to avoid zero eigenvalues. The modified eigenvalues are:

\[
\begin{align*}
\hat{\lambda}_1 &= \hat{\lambda}_2 = \hat{\lambda}_3 = \hat{\lambda}_6 = \max(\hat{\lambda}_1, V_\sigma) \\
\hat{\lambda}_{4,5} &= \max(\hat{\lambda}_{4,5}, V_\sigma)
\end{align*}
\]  

(4.39)

where \( \sigma \) is the spectral radius of the flux Jacobian matrix \( \mathbf{A} \). We use \( V_1 = 0.025 \) and \( V_n = 0.25 \) (Zingg et al., 2000) for the present study. In evaluating \( \mathbf{A} = \mathbf{M}_\xi \hat{\mathbf{A}}_\xi \mathbf{M}_\xi^{-1} \), Roe Average is used since a large density-gradient exists.

The scalar dissipation model developed by Jameson, Schmidt and Turkel (1981) is a simpler version of the matrix dissipation model. In the scalar dissipation model, the modified eigenvalues are given as:

\[
\begin{align*}
\tilde{\lambda}_1 &= \tilde{\lambda}_2 = \tilde{\lambda}_3 = \tilde{\lambda}_4 = \tilde{\lambda}_5 = \tilde{\lambda}_6 = \sigma
\end{align*}
\]  

(4.40)

Then Eq. 4.32 can be written as:

\[
d_{i+1/2,j,k}^{(2)} = \xi_{i+1/2,j,k}^{(2)} \left[ \frac{\partial \mathbf{Q}}{\partial \xi} \right]_{i+1/2,j,k} - \xi_{i+1/2,j,k}^{(4)} \left[ \frac{\partial^3 \mathbf{Q}}{\partial \xi^3} \right]_{i+1/2,j,k}
\]  

(4.41)
The matrix dissipation model is more generalized and accurate, although the computation of these matrices at every grid-cell requires more computational time and memory.

The second-difference dissipation term given in Eq. 4.32 and Eq. 4.41 is nonlinear. Its purpose is to introduce an entropy-like condition and to suppress oscillations in the neighborhood of shock discontinuities. This term is small in the smooth portion of the flow field. The switch \( \nu_{i,j,k} \) is important near discontinuities, since there are large pressure-gradients across them. For resolving flames, however, this switch is changed to include temperature- or density-gradients, as pressure may still be uniform across the flame. The fourth-order term is basically linear and is included to damp high-frequency modes and allow the scheme to approach a steady state. Only this term affects the linear stability of the scheme. Near discontinuities it is reduced to zero.

4.3 Temporal Integration: Runge-Kutta Scheme

A fourth-order Runge-Kutta (RK4) scheme is used to solve the governing equations due to its higher temporal accuracy and relatively larger CFL number (i.e., \( 2\sqrt{2} \) for a Euler calculation using RK4). A thorough investigation of the stability characteristics of the RK4 method, based on convection of the turbulence energy-spectrum, has been performed by Apte and Yang (2001) to establish its creditability and accuracy. The governing equation in the general coordinates can be rewritten as:

\[
\Delta Q = \mathbf{H} \cdot \Delta t - \Delta t \left[ \left( \mathbf{E}_5 - \mathbf{E}_5^{i+1/2,j,k} \right) \left[ u_{i-1/2,j,k} \right] + \left( \mathbf{F}_5 - \mathbf{F}_5^{i+1/2,j,k} \right) \left[ u_{i,j-1/2,k} \right] + \left( \mathbf{G}_5 - \mathbf{G}_5^{i,j,k+1/2} \right) \left[ u_{i,j,k-1/2} \right] \right] \tag{4.42}
\]

Using the four-stage Runge-Kutta scheme, each temporal-integration is completed through four consecutive intermediate steps, as given below.
\[ Q_0 = Q^n \]
\[ Q_1 = Q_0 + \alpha_1 \Delta t \cdot R(Q_0) \]
\[ Q_2 = Q_0 + \alpha_2 \Delta t \cdot R(Q_1) \]
\[ Q_3 = Q_0 + \alpha_3 \Delta t \cdot R(Q_2) \]
\[ Q^{n+1} = Q_0 + \Delta t \cdot R(Q_3) \]

where

\[ R(Q) = H - [\left( E_i^\xi - E_{i-1/2,j,k}^\xi \right) u_i,j+1/2,k + \left( F_i^\eta - F_{i-1/2,j,k}^\eta \right) u_{i,j+1/2,k} + \left( G_i^\phi - G_{i-1/2,j,k}^\phi \right) u_{i,j,k+1/2}] \]

Superscripts ‘\( n \)’ and ‘\( n+1 \)’ stand for the solution at the ‘\( n \)th’ and ‘\( n+1 \)th’ time steps, respectively.

Evaluation of the \( \Delta Q = Q^{n+1} - Q^n \) term in Eq. 4.17 is thus performed as explained above. The coefficients \( \alpha_1 \), \( \alpha_2 \), and \( \alpha_3 \) can be varied to obtain a variety of schemes with different stability properties. The standard four-stage scheme has the following values (Jameson, 1983):

\[ \alpha_1 = \frac{1}{4}, \quad \alpha_2 = \frac{1}{3}, \quad \alpha_3 = \frac{1}{2} \]

In order to enhance numerical efficiency and minimize the complexity arising from the irregular shape of the computational mesh, a curvilinear coordinate transformation of the governing equations is employed so that the grid spacing in the transformed domain is unity. This is equally important for the use of spatial filtering in the LES technique. Non-uniform filter sizes directly violate the assumptions behind the filtering approach. One has to apply the numerical methodology in the body-fitted coordinate system.
4.4 Characteristic Boundary Conditions

At the inlet and exit boundary, care must be taken when specifying the numerical boundary conditions. One has to ensure that the unphysical spurious wave reflections are avoided at the boundary and the flow is capable of relaxing to ambient conditions in prescribed ways, which can be satisfied using the Methods of Characteristic (MOC) proposed by Thompson (1987, 1990) and by Poinsot and Lele (1992). In the absence of a significant diffusion process, the MOC method provides the correct number of conditions that must be specified, as well as well-conditioned information from within the interior domain. The system of the three-dimensional Euler equations in generalized coordinates can be recast into the following form:

\[
\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{Q}}{\partial \xi} + \mathbf{B} \frac{\partial \mathbf{Q}}{\partial \eta} + \mathbf{C} \frac{\partial \mathbf{Q}}{\partial \zeta} = 0 \tag{4.46}
\]

with Jacobian matrix

\[
\mathbf{A} = \frac{\partial \mathbf{E}_\xi}{\partial \mathbf{Q}}, \quad \mathbf{B} = \frac{\partial \mathbf{F}_\eta}{\partial \mathbf{Q}}, \quad \mathbf{C} = \frac{\partial \mathbf{G}_\zeta}{\partial \mathbf{Q}} \tag{4.47}
\]

Multiplying Eq. 4.46 by left eigenvector of matrix \( \mathbf{A}, \mathbf{M}_{\xi}^{-1} \), yields:

\[
\mathbf{M}_{\xi}^{-1} \frac{\partial \mathbf{Q}}{\partial t} + \Lambda_{\xi} \mathbf{M}_{\xi}^{-1} \frac{\partial \mathbf{Q}}{\partial \xi} + \mathbf{M}_{\xi}^{-1} \left( \frac{\partial \mathbf{F}_\eta}{\partial \eta} + \frac{\partial \mathbf{G}_\zeta}{\partial \zeta} \right) = 0 \tag{4.48}
\]

To simplify the problem, we only consider a one-dimensional flow and neglect the last term of Eq. 4.48. A new vector \( \mathbf{V} \) is defined as \( d\mathbf{V} = \mathbf{M}_{\xi}^{-1} d\mathbf{Q} \). Eq. 4.48 can be written in terms of \( \mathbf{V} \) as follows:

\[
\frac{\partial \mathbf{V}}{\partial t} + \Lambda_{\xi} \frac{\partial \mathbf{V}}{\partial \xi} = 0 \tag{4.49}
\]

Eq. 4.49 can be rewritten as
\[ \frac{\partial \mathbf{V}}{\partial t} + \Gamma = 0 \]  
\[ (4.50) \]

where \( \Gamma = \mathbf{A}_v \frac{\partial \mathbf{V}}{\partial \xi} \). Eq. 4.49 is a set of wave equations for waves with characteristic velocity \( \lambda_i \) (see Eq. 4.38). For the subsonic inlet, there is only one outgoing characteristic wave. For subsonic outlet, there is only one incoming wave. A perfectly nonreflecting boundary condition requires that the amplitude of the incoming wave must be independent of time at the boundary, \textit{i.e.}, no incoming wave. Mathematically, this condition can be expressed as:

\[ \left. \frac{\partial \mathbf{V}}{\partial t} \right|_{\text{boundary}} = -\Gamma = 0 \text{ for incoming waves} \]  
\[ (4.51) \]

The outgoing waves depend only on information at and within the boundary and the \( \Gamma_i \)'s corresponding to outgoing waves in Eq. 4.48 may be calculated using one-sided differences. However, sometimes when perfectly non-reflecting boundary conditions are used, surrounding information, such as far field pressure, is lost. Corrections may be added to the treatment of boundary conditions to make them only partially non-reflecting. For subsonic outlet boundary conditions, a simple way (Rudy and Strikwerda, 1980; Poinsot and Lee, 1992) to ensure well-posedness is to set:

\[ \Gamma_5 = K \left| \mathbf{S}_\xi \right| \left( \frac{p - p_\infty}{\rho} \right) \]  
\[ (4.52) \]

where \( \Gamma_5 = (U - C)[\frac{1}{\rho c} \frac{\partial p}{\partial \xi} - (\mathbf{S}_\xi \frac{\partial u}{\partial \xi} + \mathbf{S}_\xi \frac{\partial v}{\partial \xi} + \mathbf{S}_\xi \frac{\partial w}{\partial \xi})] \). Here \( U = \mathbf{S}_\xi u + \mathbf{S}_\xi v + \mathbf{S}_\xi w \),

\[ C = \left| \mathbf{S}_\xi \right|, \ K = \sigma(1 - M^2)c / L_c \ (M \text{ represents the maximum Mach number in the computational domain).} \] \( L_c \) is the characteristic axial length of the domain in generalized coordinates, \( c \) is the local speed of sound, and \( \sigma \) is a constant ranging from 0.25 to 0.5 (Poinsot and Lele, 1992; Baum et al., 1994).
Constant pressure subsonic outflow boundary conditions are also proposed by Thompson (1987, 1990) and by Poinsot and Lele (1992) using MOC. The Local One Dimensional Inviscid (LODI) relations suggest that:

\[
\Gamma = -\Gamma_4
\]  

(4.53)

The general form for the boundary condition can be written as

\[
M^{-1}_\xi \hat{\frac{\partial}{\partial t} Q} + \Gamma + M^{-1}_\xi \left( \frac{\partial F}{\partial \eta} + \frac{\partial G}{\partial \zeta} \right) = 0
\]

(4.54)

Equation 4.48 can be discretized in the following using the Runge-Kutta scheme

\[
M^{-1}_\xi (Q^i - Q^n) = -\Delta t \alpha_i \{ \Gamma + M^{-1}_\xi \left( \frac{\partial F}{\partial \eta} + \frac{\partial G}{\partial \zeta} \right)(Q^{i,1}) \}
\]

(4.55)

where \( i = 1, 2, \ldots, N \) represents the \( N \)-step Runge-Kutta scheme. For a subsonic outflow condition, Eq.4.53 can be rewritten as:

\[
M^{-1}_\xi (Q^i - Q^n) = -L^+ \Delta t \alpha_i \{ M^{-1}_\xi \left( \frac{\partial E}{\partial \xi} + \frac{\partial F}{\partial \eta} + \frac{\partial G}{\partial \zeta} \right)(Q^{i,1}) \}
\]

(4.56)

\[
- L^- \Delta t \alpha_i \{ \Gamma + M^{-1}_\xi \left( \frac{\partial F}{\partial \eta} + \frac{\partial G}{\partial \zeta} \right)(Q^{i,1}) \}
\]

where \( L^+ \) and \( L^- \) are selection matrices

\[
L^+ = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
\end{bmatrix}
\]

and \( L^- = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix} \)
4.5 Re-Initialization Process

The method described by Sussman et al. (1994) and Russo et al. (2000) is used here to ensure the condition \(|\nabla \tilde{G}| = 1\) and to keep the level-set function as a signed distance outside the flame front. The following partial differential equation is solved iteratively to steady state:

\[
\begin{align*}
\frac{\partial \tilde{G}}{\partial \tau} &= \text{sgn}(\tilde{G}^0)(1 - |\nabla \tilde{G}|) \\
\tilde{G}(x,0) &= \tilde{G}^0(x)
\end{align*}
\]  

(4.57)

where \(\text{sgn}(\tilde{G}^0)\) is a sign function. This equation is a so-called Hamilton-Jacobi type equation.

Using coordinates transformation from \((x, y, z)\) to \((\xi, \eta, \zeta)\):

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

(4.58)

Eq. 4.57 can be written as:

\[
\begin{align*}
\frac{\partial \tilde{G}}{\partial \tau} &= \text{sgn}(\tilde{G}^0)(1 - (\alpha \frac{\partial \tilde{G}}{\partial \xi})^2 + \beta(\frac{\partial \tilde{G}}{\partial \eta})^2 + \gamma(\frac{\partial \tilde{G}}{\partial \zeta})^2 \\
&+ l(\frac{\partial \tilde{G}}{\partial \xi} \frac{\partial \tilde{G}}{\partial \eta} + m(\frac{\partial \tilde{G}}{\partial \xi} \frac{\partial \tilde{G}}{\partial \zeta}) + n(\frac{\partial \tilde{G}}{\partial \eta} \frac{\partial \tilde{G}}{\partial \zeta}))^{1/2})
\end{align*}
\]  

(4.59)

where

\[
\begin{align*}
\alpha &= \xi_x^2 + \xi_y^2 + \xi_z^2; \quad \beta = \eta_x^2 + \eta_y^2 + \eta_z^2; \quad \gamma = \zeta_x^2 + \zeta_y^2 + \zeta_z^2 \\
l &= 2(\xi_x \xi_y + \xi_x \xi_z + \xi_y \xi_z); \quad m = 2(\xi_x \eta_x + \xi_y \eta_y + \xi_z \eta_z); \quad n = 2(\xi_x \zeta_x + \xi_y \zeta_y + \xi_z \zeta_z)
\end{align*}
\]
An upwind approximation, which is motivated by the hyperbolic conservation laws, is used for space discretization. Define

\[ a = D^i \tilde{G}_{i,j,k} = \frac{\tilde{G}_{i,j,k} - \tilde{G}_{i-1,j,k}}{\Delta \xi} \quad (4.60) \]

\[ b = D^i \tilde{G}_{i,j,k} = \frac{\tilde{G}_{i+1,j,k} - \tilde{G}_{i,j,k}}{\Delta \xi} \quad (4.61) \]

and

\[ \frac{\partial \tilde{G}}{\partial \xi} = \begin{cases} \max(a,-b,0) & \text{if } (\tilde{G}^0_{i,j,k} > 0) \\ \max(-a,b,0) & \text{if } (\tilde{G}^0_{i,j,k} < 0) \end{cases} \quad (4.62) \]

Similar approximations can be used in the \( \eta \) and \( \zeta \) directions. The reasoning behind using upwind approximation for the Hamilton-Jacobi equation can be naturally understood from the perspective of the propagating wave direction and characteristics. For numerical purposes, it is useful to smooth the sign function \( \text{sgn}(\tilde{G}^0) \). We can achieve this by defining

\[ \text{sgn}(\tilde{G}^0) = \frac{\tilde{G}^0}{\sqrt{(\tilde{G}^0)^2 + \varepsilon^2}} \quad (4.63) \]

where \( \varepsilon \) is a tunable parameter that determines the sizes of the bandwidth of numerical smearing. A typical value is \( \varepsilon = \Delta \eta^{1/3} \). Because we only need the level-set to be a distance function near the flame front \( \tilde{G} = 0 \), it is not necessary to solve Eq. 4.58 to steady state over the whole domain.

The so-called narrow banding strategy (Sethian, 1999) is used here to avoid unnecessary calculation far away from the flame front and to improve computational efficiency. A second order TVD Runge-Kutta method (Gottlieb and Shu, 1998) is used for time discretization. During our calculation, the level-set \( \tilde{G} = 0 \) is used as boundary conditions. Since all of the information propagates outward from \( \tilde{G} = 0 \) surface, boundary conditions do not have to be specified on the
lateral boundary of the domain. A more detailed description of level-set methods can be found in Sethian (1999).

4.6 Flamelet Library

In the flamelet library approach, the calculation of the chemical process is decoupled from the turbulent flow calculation. Before flow computation, a family of laminar flamelets are first obtained, which gives the temperature and species-concentration distribution at different unburned gas temperature, equivalence ratio and pressure etc. Then, the filtered values of temperature and species-concentration are calculated using the Presumed PDF method and stored as flamelet libraries. During computation, the flow solver retrieves the relevant data from the libraries for each grid point.

4.6.1 Chemistry Solver

As stated in chapter 3, a system of transport equations for the one-dimensional freely propagating, laminar flame is solved here to obtain the flamelet libraries. The CHEMKIN Premix code developed by Kee et al. (1992) is used in the present study for this purpose. In the Premix code, finite difference discretization and the Newton method are employed to solve the boundary value problem on an adaptive grid. The program runs in conjunction with two preprocessors (CHEMKIN Gas-phase Interpreter and Transport Property Preprocessor) for the chemical reaction mechanisms and the transport properties. Different chemical reaction mechanisms can be applied. In this work, the GRI-MECH 3.0 mechanism (Smith et al.) for methane and air, which consists of 325 elementary reactions and 53 species, is used. The resulting temperature and species-concentration distribution are stored as a function of the distance to flame front,
while the flame front corresponds to the location of $CO_{max}$. The laminar flame speed can also be obtained using the CHEMKIN Premix code.

### 4.6.2 PDF Integration

The PDF integration can either be performed before the flow computation or during the flow computation. The latter, however, needs to be done on every grid point at each time step, which makes the computation time-consuming. Hence, we perform the PDF integration before the flow computation. Eq. 3.68 can be rewritten as:

$$\tilde{Y}(x, t) = \int_{-\infty}^{\infty} Y_n(G) \frac{1}{[2\pi(G^{n^2})_0]^{1/2}} \exp\left[-\frac{(G - \tilde{G}(x, t))^2}{2(G^{n^2})_0}\right] dG$$

Eq. 4.64 states that the filtered values of temperature and species-concentration can be expressed as a function of $\tilde{G}$ and $G^{n^2}$. Thus, a family of two-dimensional flamelet libraries (at different unburnt gas temperature, equivalence ratio and pressure etc.) are built that encompasses all possible $\tilde{G}$ and $G^{n^2}$ values encountered in the actual flow calculation.

The coupling of the flow equations and the flamelet library is treated following the approach used by Herrmann (2000). During the computation, the flow solver does not retrieve directly the temperature and species-concentration, it only considers the net effect of chemical reaction on turbulent flow field. The thermophysical variables extracted from the flamelet library are the ratio of specific heats $\gamma$, the gas constant $R$, and the enthalpy of formation of mixture

$$\psi = \sum_{k=1}^{N} Y_k \Delta h^0_{f,k}.$$  The temperature is determined through Eq. 3.32 using the preceding three variables and other flow properties obtained from the flow equations. Heat release is also obtained from the flamelet library.
4.7 Parallel Implementation

4.7.1 Parallel Architecture

Every computer, whether sequential or parallel, operates by executing instructions on data. Depending on whether there is one or several instruction streams and data streams, the computing architecture can be classified into four categories (Flynn, 1966).

1. Single Instruction stream, Single Data stream (SISD)
2. Multiple Instruction streams, Single Data stream (MISD)
3. Single Instruction stream, Multiple Data stream (SIMD)
4. Multiple Instruction stream, Multiple Data stream (MIMD)

SISD computers are the standard sequential computer with single processor. In MISD computers, each processor has its own control unit, but they share a common memory. However, MISD machines are seldom used in practice. For SIMD computers, all processors operate under the control of a single instruction stream. TMC CM-200, MasPar, ICL DAP can be regarded as SIMD machines. However, the most widely used computing architecture is the MIMD system, which is indicated schematically in Fig. 4-4. In this configuration, each processor has its own data set as well as a set of instructions to follow. These processors work independent of each other on these data sets and only communicate at some point during the computation where the data set and the results obtained are shared by two or more processors. MIMD-type computers include IBM SP-2, Cray T3E, CM5 and Beowulf Clustered computers.

For the SIMD or MIMD systems, it is usually necessary to exchange data between processors. This can be done in two ways: 1) shared memory systems, and 2) Distributed memory systems. The shared memory system consists of global address space, which is accessible by all processors and thus memory is shared among these processors. One processor
can communicate with other processors by writing into or reading from the global memory. This architecture inherently solves the inter-processor communication problem, but introduces bottleneck problems created from simultaneous access to the memory by more than one processor. In the distributed memory systems, each processor has its own local (or private) memory and the global/shared memory is absent. The processors are connected externally to switches and a network of wires to allow communications among them. The efficiency of these systems is based on the communication time required among these processors, however, and enjoys several advantages such as hardware compatibility, functionality, and performance. The only drawback of this architecture is the enormous responsibility placed on software programmers. The programmers must provide an efficient scheme to distribute the data and set of instructions, and also explicitly provide the instruction set for communications among the various CPUs. This requires reconstruction of the numerical algorithm and synchronization of the processors for efficient, parallel computing.

Fig. 4-4: Multiple instruction multiple data (MIMD) architecture (adopted from Apte, 2000)
4.7.2 Beowulf Cluster Parallel Computers

A Beowulf system is a multi-computer architecture used for parallel computations. In a Beowulf system, one server computer and many other client computers are connected together via high-speed networks. It is a distributed memory, MIMD system built primarily using commodity hardware components, such as any PC capable of running the free operating system Linux, standard Ethernet adapters, and switches. The first Beowulf system was built by Donald Becker in 1994, and consisted of 16 486DX4-100MHz machines each with 16 MB of memory. The main advantage of a Beowulf system is its high performance/price ratio in comparison with other dedicated MPP systems. Another important characteristic of the Beowulf clusters is compatibility. Changes of hardware, including the node and network system, will not affect the programming model. A Beowulf system also uses commodity software, such as the Linux operating system, Message Passing Interface (MPI) and other available open-source software.

The work conducted for this study was implemented on an in-house Beowulf system, consisting of 500 Pentium II/III processors, a Giga-Bit switch and 100MB fast Ethernet Cards. The operating system was RedHat Linux. The Message Passing Interface (MPI) involving a library of functions and macros that can be used in C, FORTRAN, and C++ Program were used to exchange the information among processors. More detailed information about this Beowulf system can be found in (Wang, 2002).

4.7.3 Domain Decomposition

Because the explicit time stepping numerical scheme (RK4) was applied in the current study, only the neighboring data instead of the data from the whole computational domain were
required during the calculation of variables in each cell. Since the data dependence is weak, the
domain decomposition technique is best suited for this kind of application. It is also commonly
implemented in distributed-memory parallel computer systems. In the field of computational
fluid dynamics (CFD), it is generally referred to as mesh partitioning, based on the geometric
substructure of the computational domain. In the domain-decomposition technique, the physical
domain is divided into several sub-domains. Variables in each cell are updated to the next time
step simultaneously. In order to calculate the spatial derivatives at the sub-domain boundaries,
ghost cells or halo data around the computing cells are introduced. Fig. 4-5 shows an example of
a two-dimensional sub-domain with ghost cells. Because the variables in the ghost cell are
updated in another sub-domain, message passing is required to synchronize data between
different sub-domains. The communication overhead is directly proportional to the volume-to-
surface ratio of the grid system in that sub-domain. Maximizing the computation-to-
communication ratio leads to higher parallel execution efficiency.

![Figure 4-5](image)

Fig. 4-5: Schematic of a two-dimensional sub-domain with ghost cells (adopted from Wang, 2002)
Chapter 5

Bifurcation of Flame Structure from a Stable to an Unstable State

5.1 Introduction

It is well established that the flow and flame dynamics in a combustion chamber can change dramatically as the governing parameters pass through their critical values at which bifurcation points are located. Combustion processes alone may or may not exhibit bifurcation phenomena, but when they take place in the presence of nonlinear behavior of the chamber dynamics, this sort of characteristic is indeed observed in many combustion devices (Knoop et al., 1997, Broda, et al., 1998, Lieuwen, 2002). Sometimes, when bifurcation takes place, which may arise from disturbances of the governing parameters, transition from a stable operation (characterized by a limit cycle with small oscillation or no oscillation) to an unstable operation (characterized by a limit cycle with large oscillation) is observed. The self-excited large unsteady flow oscillations in combustors, which are usually referred to as combustion instability, have hindered the development of gas-turbine engines with lean premixed (LPM) combustion for many years. Understanding of the mechanisms responsible for inducing bifurcation is important for passive and active control of combustion instability (Isella, 1997, Lieuwen, 2002).

Several experimental studies have been conducted to investigate combustion dynamics with bifurcation phenomena in combustion systems. Culick and colleagues (Knoop, et al., 1997, Isella et al., 1997) investigated the hysteresis behavior of combustion instability in a dump combustor as function of mixture equivalence ratio, in which several attractors coexist for a given parameter value, and the transition from a stable to an unstable state and its reverse occur at
different critical parameter values. Lieuwen (2002) studied the limit-cycle oscillations in a gas-turbine combustor. It was suggested that cyclic variability is caused by background noise. The inlet velocity not only plays an important role in determining the stability characteristics of the combustor, but also affects the amplitudes of the oscillations.

Broda et al. (1998) performed an excellent experimental study of combustion dynamics in a swirl-stabilized gas-turbine combustor. The system consists of a single-swirl injector, an axisymmetric chamber, and a choked nozzle, as shown schematically in Fig. 5-1. Natural gas is injected radially from the center body through ten holes immediately downstream of the swirler vanes. A broad range of equivalence ratio and inlet air temperature was considered systematically. Fig. 5-3 shows stability maps as a function of inlet air temperature and equivalence ratio. Instabilities occur only when the inlet air temperature is greater than a threshold value $T_{in}^*$ around 660 K and the equivalence ratio falls into the range between 0.5 and 0.7. Fig. 5-4 shows typical photographic images of a stable and an unstable flame with an equivalence ratio 0.6. As the inlet temperature increases and exceeds the threshold value $T_{in}^*$, the flame structure transforms from a stable to an unstable state, and the amplitude of pressure oscillation increases and reaches another limit cycle.

In this chapter, the effect of inlet flow temperature on flame bifurcation phenomenon in a LPM swirl-stabilized combustor, simulating the experimental conditions reported by (Broda, 1998, Seo, 1999), will be investigated numerically. Various fundamental processes, such as high temperature mixture filling, flame trapping, and vortex flashback process, responsible for the flame transition from a stable to an unstable state are carefully identified and quantified.
5.2 Physical Model and Boundary Conditions

The physical model of concern is shown in Fig. 5-1. It includes an axisymmetric chamber connected upstream with a swirl injector and downstream with a choked nozzle, simulating the experimental facility described by (Broda, 1998, Seo, 1999). Lean premixed air and methane gases are delivered to the chamber through eight straight, flat vanes with an angle of $\varphi$ degrees relative to the incoming flow. Following common practice, the swirl number $S$ is defined as the ratio of the axial flux of the angular momentum to the product of the axial momentum flux and a characteristic radius.

$$
S = \frac{\int_{R_h}^{R_n} \bar{u} \bar{w} r^2 dr}{\int_{R_h}^{R_n} \bar{u} r^2 dr}
$$

(5.1)

where $R_h$ and $R_n$ are the radii of the center body and the inlet duct, respectively (See Fig. 5-2). If we assume the axial and azimuthal velocities are uniform and the vanes are very thin, the swirl number can be written as:

$$
S = \frac{2}{3} \left[ \frac{1 - (R_h / R_n)^3}{1 - (R_h / R_n)^2} \right] \tan \varphi
$$

(5.2)

where $\varphi$ is the swirler vane angle. Natural gas is injected radially from the center body through ten holes immediately downstream of the swirler vanes. The fuel/air mixture is assumed to be well mixed before entering the combustor. The chamber measures a diameter of 45 $mm$ and a length of 235 $mm$ through the nozzle throat. The choked nozzle at the exit prevents any downstream disturbances from traveling upstream and to maintain the desired chamber pressure. A choked venturi is also installed at the inlet entrance to acoustically isolate the test section from the air supply line.

The baseline condition includes an equivalence ratio of 0.573 and a chamber pressure of 0.463 $MPa$, The mass flow rates of the natural gas and air are 1.71 and 50.70 $g/s$, respectively.
The inlet flow velocity is 86.6 m/s and the corresponding Reynolds number based on the inlet flow velocity and height of the inlet annulus is 35000. A generic swirler with swirl angles of 45 degrees was investigated. The estimated swirl number is 0.76, which is in the category of high-swirl number (approximately $S \gtrsim 0.6$, (Gupta et al., 1984)).

The formulation is based on the Favre-filtered conservation equations of mass, momentum and energy. The SGS terms are modeled using a compressible-flow version of the Smagorinsky model suggested by Erlebacher et al. (1992) and level-set flamelet library approach is used here for the treatment of premixed turbulent combustion. Boundary conditions must be specified to complete the formulation. The no-slip and adiabatic conditions are enforced along all of the solid walls. At the inlet boundary, the mass flow rate and temperature are specified. The pressure is obtained from a one-dimensional approximation to the axial momentum equation, i.e.,

\[
\frac{\partial p}{\partial x} = -\rho \frac{\partial u}{\partial t} - \rho u \frac{\partial u}{\partial x}.
\]

The mean axial-velocity distribution follows the one-seventh power law by assuming a fully developed turbulent pipe flow. The radial and azimuthal velocities are determined from the swirler vane angle. Turbulence properties at the inlet are specified by superimposing broadband disturbances onto the mean velocity profiles. The disturbances are generated by a Gaussian-random number generator with an intensity of 15 % of the mean quantity. The nonreflecting boundary conditions proposed by Poinset and Lele (1992) is applied at the exit boundary. Because of the enormous computational effort required for calculating the flowfield in the entire chamber, only a cylindrical sector with periodic boundary conditions specified in the azimuthal direction is treated herein (see Fig. 5-5). The analysis, in spite of the lack of vortex-stretching mechanism, has been shown to be able to capture the salient features of the turbulent flowfields and unsteady flame propagation (Menon and Jou, 1991, Thibaut and Candel, 1998).

* A random walk method proposed by Morris and Long (2002) can be used to generate broadband disturbance with broader and clearly defined spectrum.
The computational domain includes the upstream half of the chamber and part of the inlet injector, as shown in Fig. 5-5. The entire grid system consists of 376x141 points along the axial and radial directions, respectively, of which 75 axial points are used to cover the inlet duct. The largest grid size falls in the inertial sub-range of the turbulent energy spectrum, based on the inlet Reynolds number. The grids are clustered in the shear-layer regions downstream of the dump plane and near the solid walls to resolve the shear-layer and near-wall gradients. The computational domain was divided into 17 blocks and the analysis was conducted on a distributed-memory parallel computer with each block calculated on a single processor.

5.3 Results and Discussion

A family of premixed methane/air flamelet libraries with unburnt gas temperature ranging from 560 K to 700 K is established using the GRI-MECH 3.0 mechanism (Smith et al.), consisting of 325 elementary reactions and 53 species. The distributions of the temperature and species-concentration fields ($T_{in} = 660$ K, $\phi = 0.573$ and $p = 0.463$ MPa) calculated by the CHEMKIN Premix code (Kee et al., 1992) are shown in Fig 3-1. The unstretched laminar flame speed as a function of fresh gas temperature is shown in Fig. 5-6. At $T_{in} = 600$ K and $T_{in} = 660$ K, the flame speed $S_L$ is 0.34 and 0.45 m/s, respectively, and the corresponding flames thickness are around 0.3 mm (flame thickness is defined as the distance over which the reduced temperature $\Theta = (T - T_{in})/(T_{product} - T_{in})$ changes from 0.01 to 0.99). The calculated flowfield shows that the magnitude of $v'/S_L$ ranges from 6.6 to 100 and that of $l/l_p$ from 2.0 to 70, where the turbulent integral length scale $l$ is approximated from the temporal correlation function based on the Taylor’s frozen-turbulence hypothesis. The flame is mostly located in the thin reaction zone in the premixed turbulent combustion regime diagram given in Fig.3-2. The flamelet assumption
employed in the present analysis is confirmed. Fig. 5-7 shows the snapshots of the temperature and distance function (black lines, $\tilde{G}$ contour after re-initialization) for a stable and an unstable flame. The desired distance functions are obtained using re-initialization process.

5.3.1 Stable Flame Dynamics

Stable flame evolution was first obtained for an inlet flow temperature of 600 $K$ (below the threshold value $T_{in}^*$ for the onset of combustion oscillation). The flame bifurcation phenomenon was then investigated by increasing the inlet air temperature from 600 to 660 $K$. The mean chamber pressure is 0.463 $MPa$. Fig. 5-8 shows the mean temperature contours and pseudo-streamlines on the $x-r$ plane based on the mean axial and radial velocity components for a stable flame. A central torodial recirculation zone (CRTZ) is established in the wake of the center body under the effects of the swirling flow. The CTRZ, a form of vortex breakdown, serves as a flame stabilization region, where hot products are mixed with the incoming mixture of air and fuel. In addition, as a result of the sudden increase in combustor area, a corner recirculation zone (CRZ) is formed downstream of the backward-facing step.

The calculated pressure and velocity fields exhibit small-amplitude fluctuations with a dominant harmonic mode at 3214 $Hz$, corresponding to the frequency of the vortex shedding from the center body. Fig. 5-9 presents the flame evolution and vortex shedding process in the upstream region of the chamber over one cycle of oscillation. The pressure and velocity are measured at the middle point of the inlet annulus exit. The phase angle $\theta$ is referenced with respect to the acoustic velocity at the interface between the inlet and combustor. The entire process is dictated by the temporal evolution and spatial distribution of the flame front, which moves back and forth under the influences of the vortical motion (indicated by the concentrated
streamlines) in the chamber. A new vortex begins to shed from the center body at \( \theta = 90^\circ \), accompanying with a higher local flow velocity. As the vortex moves downstream (\( \theta = 180^\circ - 270^\circ \)), it distorts the flame front or even produces a separated flame pocket. At the same time, the higher speed mixture pushes the flame downstream. When the vortex moves away from the flame (\( \theta = 360^\circ \)) and dissipates into small-scale structures, the flame front propagates upstream (since the higher speed mixture is convected downstream) and interacts with another incoming vortex. During this process, a new vortex appears at the corner of the center body and another cycle repeats.

5.3.2 Bifurcation of Flame Structure

The inlet air temperature has enormous effects on the flame dynamics in the system as shown in Fig. 5-10. On the one hand, when the inlet air temperature increases, for a fixed mass flow rate, the flow velocity also increases and pushes the flame downstream. On the other hand, the increased inlet air temperature leads to an increase in the flame speed, and consequently causes the flame to propagate upstream. In addition, flashback may occur near the wall due to the small local flow velocity. The combined effects of flow acceleration, flame-speed enhancement, and flashback determine the final form of the flame structure.

In the present study, as the inlet air temperature increases from 600 to 660 K, flame bifurcation takes place. The flame originally anchored in the center recirculation zone penetrates into the corner recirculation zone and flashes back. Consequently, the flame is stabilized by both the corner- and center-recirculating flows and forms a compact enveloped configuration. The flame flaps dynamically and drives flow oscillations through its influence on unsteady heat release. At the same time, the pressure oscillation increases and reaches another limit cycle with
a much larger amplitude. The entire bifurcation process can be divided into three stages: high temperature mixture filling process, flame trapping process, and vortex flashback process, as shown in Fig. 5-11, where \( t = 0 \; ms \) denotes the time at which the inlet temperature starts to increase from 600 to 660 \( K \).

Fig. 5-11 (a-c) show the high-temperature mixture filling process. As the inlet mixture temperature increases, the flow speed increases due to the decreased density for a fixed mass flow rate. As a result, the original low-temperature mixture is pushed downstream toward the flame. Although a flashback phenomenon is observed near the wall, the high temperature mixture has not reached the flame front near the wall and the flame speed remains unchanged at this stage.

Fig. 5-11 (d-e) show the flame trapping process. Once the high temperature mixture reaches the flame front, with the help of the increased flame speed, the near-wall flashback overshadows the flow acceleration effects. As a result, the flame front penetrates into the corner recirculation zone and is trapped by the local vortical motion.

In the vortex flashback process, as shown in Fig. 5-11 (f-h), the flame propagates upstream under the influence of the vortical motion. A counter-clockwise rotating vortex originally shed from the edge of the backward-facing step approaches the flame front in the corner recirculation zone and then pushes it toward the dump plane. At the same time, a small flame pocket is produced and separated from the main stream. After this vortex is convected downstream and passes through the flame, another vortex approaches and interacts with the flame. (A more detailed vortex flashback process is shown in Fig. 5-12) This process continues and eventually the fresh reactants in the corner recirculation zone are completely burnt. The flame is stabilized by both the corner- and center-recirculating flows and its overall length is substantially reduced. This situation renders the combustor more prone to instabilities according to the Rayleigh criterion, since considerable heat is released within a short distance close to the chamber head-end (i.e., the acoustic anti-node point).
Once the flame becomes unstable when the inlet flow temperature exceeds the critical value $T_{in}^*$, it becomes rather difficult to re-establish stable operation unless the inlet temperature is reduced to a level significantly lower than $T_{in}^*$. This phenomenon is commonly referred to as hysteresis, and has been experimentally observed by many researchers [see, for example, Ref.2]. The occurrence of hysteresis under the current circumstance may be explained as follows. During unstable combustion, the corner recirculation zone is filled with high temperature products and the chamber wall in this region is heated to reach the local flame temperature. To recover the stable operation, the cold flow needs not only to extinguish the flame stabilized by the corner recirculation zone through entrainment or flame liftoff, but also to offset the effects of high temperature wall, which tends to increase the local gas temperature and inhibit extinction. Consequently, a much lower inlet temperature is required to regain stable operation. Numerical simulation of the hysteresis phenomenon necessitates a refined treatment of flame extinction and wall boundary conditions, a subject for sequent research.

5.3.3 Flame Flashback and Flame Speed

In light of the above observations, we conclude that the flashback phenomenon dictates the flame bifurcation process. Flashback in premixed combustion has been the subject of a number of experimental, analytical, and numerical studies in the past. Its occurrence is usually attributed to two mechanisms. The first involves flame propagation in the boundary layer along a solid wall, where the local velocity diminishes toward the surface. The second mechanism is associated with flow reversal, which is usually caused by vortical motions or acoustic oscillations. Both mechanisms are observed in the present case.
A criterion for the occurrence of near-wall flashback was proposed by Lewis and Von Elbe (1987), who state that flashback occurs if the velocity gradient at the wall is less than the ratio of the flame speed and the quenching distance. This criterion, however, is qualitatively correct only for isothermal walls, and is not applicable for adiabatic walls due to the lack of a quenching distance. Another criterion, valid for both adiabatic and isothermal walls, was recently proposed by Kurdyumov et al. (2000). Flashback occurs if the Karlovitz number, defined as $\frac{\alpha A}{S_L^2}$, with $\alpha$ being the thermal diffusivity and $A$ the velocity gradient at the wall, is less than a critical value. Although this criterion is formulated for laminar flows, the result can be qualitatively extended to flames in turbulent boundary layers. In the present case, the flame speed increases as the inlet air temperature increases. Consequently, the flame is more prone to flashback through the wall boundary layers according to Kurdyumov’s criterion. Flashback arising from local flow reversal has also been investigated by many researchers (Thibaut and Candel, 1998, Najm and Ghoniem, 1994). Large vortical structures and turbulent flame speed play important roles in this kind of phenomenon. The latter is essential because it controls the rate of mixture consumption.

For lean-premixed combustion, the laminar flame speed $S_L$ increases with an increase in the equivalence ratio $\phi$. Thus, increases in the equivalence ratio and inlet temperature exert similar effects on the flame evolution. However, the chemical reaction rate and heat release are much more sensitive to variations in the equivalence ratio under lean conditions than stoichiometric conditions. Moreover, near the lean blowout limit, perturbations in the equivalence ratio $\phi$ can cause periodic extinction of the flame. As a result, the equivalence ratio oscillation under lean conditions is prone to inducing flow oscillation (Lieuwen, 2002) and subsequently increases turbulent velocity fluctuation $v'$. This suggests that a lean premixed turbulent flame is more susceptible to flashback, since the turbulent flame speed $S_T$ increases not only with the laminar flame speed $S_L$, but also with turbulent velocity fluctuation $v'$. 
(Lipatnikow and Chomiak, 2002). The result helps explain why the transition from a stable to an unstable state only occurs when the equivalence ratio falls in the range between 0.5 and 0.7 (Broda, 1998)

Since the flame bifurcation is largely determined by the flashback phenomenon in the corner recirculation zone in the present case, one effective way to avoid its occurrence is to inject cold flow into that region. This procedure suppresses the local flame upstream propagation and consequently leads to a much more stable system.
Fig. 5-1: Schematic of a model swirl-stabilized gas-turbine combustor (after Seo, 1999)

Fig. 5-2: Schematic of top and cross-section views of a flat vane swirler (after Seo, 1999)
Fig. 5-3: Stability maps as a function of inlet air temperature and equivalence ratio (after Seo, 1999)
Fig. 5-4: Top: photographic images of stable and unstable flames; Bottom: pressure-time trace (after Seo, 1999)
Fig. 5-5: Schematic of 2D axi-symmetric grid system (376x141), the presented grid has fewer points than these used in the calculations, but the distributions of grid points are similar.

Fig. 5-6: Laminar flame speed as a function of fresh gas temperature
Fig. 5-7: Contour of temperature and distance function (black lines) of a stable flame (top) and an unstable flame (bottom)

Fig. 5-8: Mean temperature contours and streamlines of stable flame
Fig. 5-9: Stable flame evolution over one cycle of oscillation (3214 Hz): temperature contours and streamlines
Fig. 5-10: Effect of inlet air temperature on flame dynamics.
Fig. 5-11: Transition from stable to unstable flame with increased inlet temperature from 600 K to 660 K
Fig. 5-12: Vortex and flame interaction
Chapter 6

Unstable Flame Dynamics

6.1 Problem Description

Combustion instabilities result from the coupling between transient combustion processes and acoustic motions. Although the energy needed to drive unsteady motions is only an exceedingly small fraction of the heat release from combustion (Culick and Yang, 1992; Culick and Yang, 1997), combustion instabilities cannot be sustained unless a certain dynamic relation (the so-called Rayleigh criterion) between heat release fluctuations and acoustic pressure oscillations is satisfied in the combustion chamber. A variety of physical processes, such as equivalence ratio fluctuations, vortex shedding, and flame surface variations, may be involved in the development of instabilities depending on the system characteristics and operating conditions (Candel, 2002). When combustion instabilities take place, an energy feedback loop usually will be formed among these physical processes through acoustic motions, which propagate downstream and upstream. The objective of this chapter is to investigate the combustion dynamics in a model lean-premixed swirl-stabilized combustor under unstable operating conditions, with special emphasis placed on the key physical processes responsible for driving combustion instabilities.

In this chapter, a three-dimensional numerical analysis, with the theoretical and numerical framework described in the preceding sections, is performed to investigate the unstable flame dynamics of the lean-premixed swirl-stabilized combustor (Broda et al., 1998; Seo, 1999), as shown in Fig. 5-1. The baseline condition includes an equivalence ratio of 0.573 and a
chamber pressure of 0.463 MPa. The mass flow rates of methane and air are 1.71 and 50.70 g/s, respectively. The inlet flow velocity is 86.6 m/s and the corresponding Reynolds number based on the inlet flow velocity and height of the inlet annulus is 35000. According to the experimental observations, the combustor becomes unstable and exhibits strong flow oscillations when the inlet air temperature exceeds a threshold value and the equivalence ratio falls into the range between 0.5 and 0.7. Thus, an inlet temperature of 660 K corresponding to the case of unstable combustion reported in Broda et al. (1998) and Seo (1999) is used here.

6.2 Boundary Conditions and Computational Domain

The dominant acoustic motion in the axial direction corresponds to the first longitudinal mode (Broda, et al., 1998, Seo, 1999), with the existence of an acoustic pressure node at the middle of the chamber. Accordingly, the computational domain shown in Fig. 6-1 only includes the upstream half of the chamber and the portion of the inlet annulus downstream of the swirl vane, to save computational resources.

At the inlet boundary, the mass flow rate and temperature are specified. The pressure is obtained from a one-dimensional approximation to the axial momentum equation, i.e.,

\[ \frac{\partial p}{\partial x} = -\rho \frac{\partial u}{\partial t} - \rho u \frac{\partial u}{\partial x}. \]

The mean axial-velocity distribution follows the one-seventh power law by assuming a fully developed turbulent pipe flow. The radial and azimuthal velocities are determined from the swirler vane angle. Turbulence properties at the inlet are specified by superimposing broadband disturbances with an intensity of 15% of the mean quantity onto the mean velocity profiles. Since the acoustic oscillations generated in the chamber propagate upstream through the swirler, care must be exercised in specifying the acoustic boundary conditions at the inlet of the computational domain. The inlet venturi is choked and
basically serves as an acoustic damper that can effectively dissipate disturbances arising from downstream (Broda, et al., 1998). Consequently, the acoustic field in the inlet section is dominated by an upstream-running wave. In the present study, an acoustic admittance function defined as

\[ \hat{A}_d(\omega_n) = \frac{\hat{u}_{a,n}(\omega_n)}{\hat{p}_{a,n}(\omega_n)} / \sqrt{\rho} \]  

(6.1)

is used to characterize the response of the swirler to downstream disturbances. The instantaneous pressure and axial velocity contains contributions from the mean, turbulent, and acoustic flowfields, i.e., \( p = \bar{p} + p'_i + p'_a \) and \( u = \bar{u} + u'_i + u'_a \). The acoustic pressure can be written as:

\[ p'_a(t) = \sum_{1}^{L} \text{Re}\{ \hat{\rho}_{a,n}(\omega_n) e^{i\omega_n t} \}, \]

and the corresponding acoustic velocity can be written as:

\[ u'_a(t) = (\bar{c} / \sqrt{\rho}) \sum_{1}^{L} \text{Re}\{ \hat{A}_d(\omega_n) \hat{\rho}_{a,n}(\omega_n) e^{i\omega_n t} \}, \]

where the admittance function \( \hat{A}_d(\omega_n) \) can be obtained from an impedance-tube experiment for the swirler (Broda, et al., 1998). Generally, only a few dominating acoustic waves (which usually are the lowest order longitudinal modes) can travel upstream and need to be taken into account. In the present case, only the acoustic wave corresponding to the first longitudinal mode of the main chamber is considered because of its prevalence in the inlet.

At the outlet boundary, the characteristic conditions proposed by Poinsot and Lele (1992) are applied, along with the specification of a time-invariant back pressure due to the existence of an acoustic pressure node at the middle of the chamber. This back pressure is obtained using a simplified one-dimensional momentum equation \( \frac{\partial p}{\partial r} = \rho U_0^2 / r \) in the radial direction, where \( U_0 \) is the mean azimuthal velocity. The pressure at \( r = 0 \) is fixed as a pre-specified value. Finally, no-slip and adiabatic conditions are enforced along all of the solid walls.
The entire grid system has $176 \times 141 \times 81$ (2.01 million) points along the axial, radial, and azimuthal directions, respectively, of which 36 axial points are used to cover the inlet section. The axial and radial grids are clustered in the shear-layer regions downstream of the dump plane and near the solid walls, as shown in Fig. 6-2. The azimuthal grids are uniformly distributed. This grid resolution is chosen based on the inlet Reynolds number such that the largest grid size falls in the inertial sub-range of the turbulent energy spectrum. The analysis is conducted on an in-house distributed-memory parallel computer. The computational domain is divided into 68 blocks, and each block was calculated on a single processor, i.e., a total number of 68 processors are used.

6.3 Results and Discussion

The calculation is initiated by imposing broadband velocity fluctuations at the inlet, and continued for an extended period of time until statistically meaningful data was obtained. Fig. 6-4 shows the frequency spectra of the turbulent kinetic energy at three different locations along the inlet axis. The $-5/3$ law of energy spectrum based on the Kolmogorov-Obukhow theory, which characterizes the inertial sub-range, is largely satisfied. In LES, the cutoff wave number for turbulent motions should lie in the inertia sub-range of the kinetic energy spectrum. The result further confirms the adequacy of the numerical grid resolution achieved.
6.3.1 Unstable Flow Structures

6.3.1.1 Mean Flowfield

The mean flow properties are first obtained by taking long-time average of the instantaneous quantities. In spite of significant flow motions in the azimuthal direction, the mean flowfield remains perfectly axisymmetric (Panda and McLaughlin, 1994). Fig. 6-5 shows the mean temperature field and the pseudo-streamlines pattern on the $x-r$ plane based on the mean axial and radial velocity components. A central toroidal recirculation zone (CTRZ), a form of vortex breakdown, is established in the wake of the center body under the effects of the swirling flow. It serves as a flame stabilization region where hot products are mixed with the incoming mixture of air and fuel. In addition, as a result of the sudden enlargement of the combustor configuration, a corner recirculation zone (CRZ) with two separation bubbles is formed in the downstream of backward-facing step. The sizes of the CRZ and CTRZ are strongly dependent on the swirl intensity, equivalence ratio, and combustor geometry (Wang, 1997).

Fig. 6-6 shows the radial distributions of the mean velocity components, pressure, and turbulent kinetic energy ($tke$) at various axial locations, where $r = 0$ corresponds to the centerline of the chamber. High swirling flow is delivered to the chamber through the inlet annulus, and decays rapidly due to the flow expansion, diffusion, and viscous dissipation. The incoming flow from the inlet annulus spreads away from the centerline under the effects of centrifugal force. Strong radial pressure gradients then arise and a low-pressure region is formed in the vicinity of the center body. As the result, a negative axial velocity region appears and a recirculation flow is established in the form of CRTZ. The radial distribution of the turbulent kinetic energy indicates that a high turbulence intensity region exists in the wake of the center body, where large velocity
fluctuations are produced due to strong turbulent mixing between the incoming flow and the recirculating flow in the CTRZ.

### 6.3.1.2 Instantaneous Flowfield

Vorticity is of concern in the present study because of its dominant influence in determining the flow entrainment in the reaction zone and the subsequent flame evolution. Fig. 6-7 shows a snapshot of the vorticity field on the $x-r$ and $r-\theta$ planes. Large vortical structures arise in the shear layer downstream of the dump plane and around the wrinkled flame zone. In addition to the swirler-induced vorticity, the volume dilation and baroclinic effects in the flame zone contribute significantly to the production of vorticity. Vorticies are convected downstream with accompanying irregular breaking strength (i.e., vortex breakdown), and spiral into the core region. This precessing vortex core (PVC) induces strong flow oscillations, and may even resonate with the acoustic instability in the chamber.

The phenomenon of vortex breakdown, defined as an abrupt change in the character of a vortex core, is manifested with the recirculation zone in the downstream of the center body. The region provides the mechanisms for flame stabilization, and is characterized by the existence of internal stagnation points and reversed flows. Lucca-Negro and O’Doherty (2001) listed seven different types of vortex breakdown. Among them, bubble and spiral modes of breakdown are commonly observed in swirl-stabilized gas-turbine combustors. The bubble mode usually prevails at high swirl numbers, while the spiral mode dominates at low swirl numbers.

Fig. 6-8a shows the iso-surface of the vorticity field at $\omega = 75000 \, l/s$. The flow-field in the region of $r > 2 \, cm$ is blanked to provide a clear picture of the flow structures. A vortex spiral evolves from the shear layer originating at the backward facing step due to the Kelvin-Helmholtz instabilities in both the axial and azimuthal directions (Coats, 1996). This single tilted
spiral-like structure gyrates around the centerline and persists for about two turns before breaking up into small-scale structures. The winding of the spiral is in the direction opposite to the swirling flow, which is consistent with the argument of Martin and Meiburg (1996) that the counter-rotating helical waves are much more unstable in swirling flows. There still, however, remain some controversial opinions about the orientation of the spiral. The winding of the spiral has been observed to occur either in the sense of the rotation of the swirling flow, or opposite to it. No definite theory has been provided so far to explain this discrepancy (Lucca-Negro and O’Doherty, 2001).

Fig. 6-8b shows the iso-surface of the vorticity field at $\omega = 75000$ $l/s$ with the region of $r > 1$ $cm$ blanked. An asymmetric bubble-like structure is observed with its stagnation point approaching the centerbody. It is difficult to identify a succinct structure due to the complex flow pattern. Both spiral and double helix structures are evidenced in connection with the existence of a precessing vortex core. According to Brucker (1993), the bubble and spiral modes of breakdown appear to be very similar, and the former can be regarded as a ‘compressed’ spiral.

Swirling flows are often non-axisymmetric and unstable. A phenomenon called precessing vortex core (PVC) exists when a central vortex core starts to precess around the axis of symmetry due to the helical instability. Although the PVC may benefit combustion efficiency through its enhancement of turbulence intensity and mixing, it represents largely an undesired characteristic because of the resonant coupling with low-frequency acoustic oscillation in the combustion chamber. In the present study, two kinds of PVC, of the spiral and double-helix modes, are observed. Fig. 6-9 shows the instantaneous streamlines on the transverse planes at three different axial locations. At $t = 11.91$ $ms$, a double helix mode of PVC is found with two vortex cores spiraling around the centerline, while at $t = 12.34$ $ms$, a single vortex core spirals around the centerline. Both the spiral and double helix wind in a direction opposite to the main swirling flow. The mechanisms for triggering the transition between these two states are still
The existence of PVC helps explain the occurrence of negative azimuthal velocity in the region near the centerline of the chamber.

6.3.2 Unstable Combustion Dynamics

6.3.2.1 Acoustic-Mode Identification

Since the most problematic type of instability involves the coupling between acoustic motions and transient combustion response, a prerequisite of any instability research is the identification of acoustic modes in the chamber. Numerous probes were employed in the present study to register the flow oscillations in the chamber. Fig. 6-10 shows the frequency content of the pressure fluctuations at two different locations immediately downstream of the dump plane. Four dominant modes at the frequencies of 1795, 6852, 10970 and 21741 Hz are clearly observed. To facilitate data analysis and to help provide physical insight, a linear analysis of the acoustic field was performed. The inlet was assumed to be filled with a premixed combustible mixture with a speed of sound of \( c = 510 \) m/s and the chamber with the burnt gases with the speed of sound of \( c = 820 \) m/s. An acoustically closed boundary was employed for the choked exit nozzle. The acoustic impedance of the swirler was tuned to match with the measured acoustic pressure distribution in the inlet annulus. The results from the linear acoustic analysis are summarized in Table 6-1.
The calculated frequency of 1795 Hz corresponds to the first longitudinal (1L) mode of acoustic oscillation in the chamber, which matches closely with the measured value of 1750 Hz (Broda, 1998). The slight deviation from the prediction of the linear acoustic analysis results from the uncertainties in specifying the averaged speed of sound and the chamber length. It is worth noting that the experimental measurements also indicate the existence of the second longitudinal (2L) mode at 3500 Hz. This mode, however, was suppressed in the present numerical study since the back pressure at the end of the computational domain was fixed at a pre-specified value, a condition that prohibited the excitation of higher modes of longitudinal oscillations. The calculated mode at 6582 Hz corresponds to the first longitudinal (1L) mode of acoustic oscillation in the inlet annulus, and the modes at 10970 Hz and 21742 Hz to the first tangential (1T) and the first radial (1R) modes of the main chamber, respectively. Fig. 6-10 also shows good agreement in acoustic mode shape between the calculated and the analytical results. The present analysis is capable of solving the acoustic wave motions in various parts of the domain.

### Table 6-1: Acoustic Frequencies Predicted by Linear Analysis

<table>
<thead>
<tr>
<th>Mode</th>
<th>1L (Hz)</th>
<th>1T (Hz)</th>
<th>1R (Hz)</th>
<th>2T (Hz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber</td>
<td>1830</td>
<td>10678</td>
<td>22226</td>
<td>17700</td>
</tr>
<tr>
<td>Inlet</td>
<td>6375</td>
<td>11065</td>
<td>48726</td>
<td>21827</td>
</tr>
</tbody>
</table>

6.3.2.2 Vortex Shedding and Acoustics Interaction

As the flow expands from the injector to the chamber, strong shear layers are formed in the downstream of the central body and backward-facing step. The inherent hydrodynamic instability and vortex shedding play a decisive role in determining the combustion dynamics in
the chamber. When the characteristic frequencies of these processes match with those of the chamber acoustic waves, intensive interactions occur and give rise to large excursions of unsteady motions through the coupling with unsteady heat release in the flame zone.

A comprehensive review of large-scale structures in shear layers has been given by Schadow and Gutmark (1992). Instability waves develop and grow in a shear layer in its initial region. When the amplified waves reach a certain energy level, they roll up into vortices. The initial vortex-shedding frequency, $f_i$, also known as the most amplified frequency, can be scaled with the initial momentum thickness $\theta_0$, and a characteristic velocity $\bar{U}$ of the shear layer. The result leads to a non-dimensional frequency or Strouhal number, $Sr_i = f_i \theta_0 / \bar{U}$. Linear instability theory for laminar mixing layers predicts this number to be close to 0.032, with $\bar{U}$ defined as the average bulk velocity $(U_1 + U_2)/2$. For a turbulent shear layer, the number changes to $Sr_i \approx 0.044 - 0.048$ (Ho and Huerre, 1984). As vortices move downstream, they merge together to oscillate at the sub-harmonics of the initial vortex shedding frequency $f_i / N$, with $N = 2, 3, 4 \ldots$. In most practical flows, this pairing process is terminated at some point by the finite extent of the bounding stream. Therefore there exists a cut-off frequency in the sequence of the sub-harmonics. For an axisymmetric jet, the frequency of the final sub-harmonic can be scaled with the initial diameter $D$ and velocity $U_0$ of the jet (Coats, 1996). The resultant preferred-mode Strouhal number is defined as: $Sr_j = f_j D / U_0$. The range of $Sr_j$ was found to be between 0.25 and 0.5. This preferred-mode frequency $f_j$ usually falls in the second or third sub-harmonic range of the initial frequency $f_i$.

Although many of the existing hydrodynamic analyses have been formulated for planar flows, they can be applied with good accuracy to mixing layers in axisymmetric configurations by assuming the shear-layer thickness is very thin compared to its radius of curvature. (Note that
there are also many instability studies of axisymmetric jets, for example, Morris, 1976, 1983). The density differences, which may arise from combustion, are found to have very limited effects on the most amplified frequency (Soteriou and Ghoniem, 1995). In the present case, the momentum thickness \( \theta_0 = \int_0^\infty \left( \frac{u}{U_{\max}} \right) (1 - \frac{u}{U_{\max}}) dy \) estimated from the calculated mean velocity field is 0.1 mm. \( \overline{U} \approx 43.3 \text{ m/s}, U_\infty \approx 86.6 \text{ m/s}, \) and \( D = (D_n - D_h)/2 = 5.385 \text{ mm}. \) If we choose \( Sr_i = f_j \theta_0 / \overline{U} = 0.048, \) then the most amplified frequency \( f_i \) is 20784 Hz. The corresponding second and third harmonic frequencies are 10392 Hz and 6928 Hz, respectively. The Strouhal number calculated from the third sub-harmonic frequency 6928 Hz using \( Sr_j = f_j D / U_\infty \) is 0.43, which is in the range of the preferred-mode Strouhal numbers. This finding suggests that the third sub-harmonic frequency is also a preferred-mode frequency. Thus, the most amplified frequency of the shear-layer instability \( (f_i = 20784 \text{ Hz}) \) matches closely to the 1R mode (21742 Hz) of acoustic oscillation in the chamber, and the second sub-harmonic frequency \( f_i/2 = 10392 \text{ Hz} \) agrees with the 1T mode (10970 Hz) of the chamber acoustic waves. Furthermore, the third sub-harmonic frequency (6928 Hz) is very close to the 1L mode (6582 Hz) of the acoustic waves in the inlet annulus. The strong resonance between the vortex shedding in the shear layer and acoustic motions leads to the excitations of the 1R and 1T modes of the chamber and the 1L mode of acoustic waves in the inlet annulus.

### 6.3.2.3 Unstable Flame Evolution

The mean temperature field shown in Fig. 6-5 clearly exhibits a double-surface envelope flame anchored at the edges of the center body and the backward-facing step. This is in sharp contrast with the flame structure under stable operating conditions that shows only a single
conical flame stabilized by the centerbody (Broda, 1998, Seo, 1999). One major factor contributing to this phenomenon is the relatively higher inlet flow temperature in the present study compared to that required for stable combustion. As the inlet temperature increases, the chemical induction time is shortened, and eventually reaches a level comparable to the flow residence time in the corner circulating zone downstream of the dump plane. A flame is thus established in that region, and merges with the one originating from the centerbody. The overall flame length is substantially reduced. This situation renders the combustor more prone to instabilities according to the Rayleigh criterion, since much heat release occurs within a short distance close to the chamber head-end (i.e., acoustic anti-node point).

The flame dynamics can be elucidated by considering its interaction with the local oscillatory flowfield. Fig. 6-11 presents the temporal evolution of the temperature field in the upstream of the chamber on the $x-r$ and $r-\theta$ planes over one cycle of the 1L mode of acoustic oscillation. The phase angle $\theta$ is referenced with respect to the acoustic pressure of the 1L mode at the chamber head-end. The entire process is dictated by the cold-flow entrainment into and mixing with hot gases in the vortical structures in the flame zone. During the pressure build-up stage (around $\theta = 0^\circ$), the increasing pressure and favorable pressure gradient near the dump plane facilitates the delivery of the fresh reactants into the chamber. Intensive heat release then occurs after a short fluid mixing and chemical induction time. The resultant flow expansion tends to push the flame outward and simultaneously block the inlet flow at the dump plane. Unburned mixture fragments may break-up away from the main stream, and generate local hot spots when they are convected downstream. In the next stage (around $\theta = 180^\circ$), the decreasing pressure and adverse pressure gradient near the dump plane prevents the fresh reactants from traveling downstream in the chamber. The flame zone is thus reduced and becomes a little more compact.
The temperature evolution in the transverse plane exhibits the three-dimensional structure of the flame and can be well correlated with the vorticity field shown in Fig. 6-7.

It should be noted that the above description of flame motion is not precisely reflected in the temperature field shown in Fig. 6-11 due to the various time delays involved in the process. The qualitative trend, however, remains valid and is consistent with distribution of Rayleigh parameter, as will be discussed later. The detailed flame dynamics can also be studied by plotting the flame surface motions. Fig. 6-13 presents the evolution of the isothermal surface at $T = 1700$ $K$ over one cycle of the 1L mode of acoustic oscillation, viewed from three different angles. The flame front is clearly contorted and convoluted by the spiral vortex structures, further revealing the interactions between the vortical field and the flame dynamics.

6.3.2.4 Vortex and Flame Interaction

The interaction between the acoustic and the shear layer instability wave motions depend on the matching of frequencies between these two types of instabilities. In the present case, the most amplified frequency of the shear layer instability wave $f_i$ (20784 Hz) is close to the 1R mode of acoustic oscillations in the chamber (21742 Hz) and the first sub-harmonic frequency $f_i/2$ (10392 Hz) to the 1T mode of the chamber (10970 Hz). Both the 1R and 1T acoustic modes are expected to interact intimately with vortex shedding. Fig. 6-14 shows the instantaneous vorticity field at various times within one cycle of the 1T acoustic oscillation. The thick black line indicates the flame front. Well-organized vortices are shed from the edge of the backward-facing step. The process, however, becomes much more complex in the downstream of the center body due to the existence of a toroidal recirculating flow. New vortices are produced at the tip of backward-facing step at $\theta = 72^0$, and bulge the flame front. They continue to distort
the flame or even produce separated flame pockets when traveling downstream. Finally, these vortices move out of the flame region and dissipate into small-scale structures. Another set of vortices appears at $\theta = 360^0$ at the dump plane, and the cycle repeats.

To further examine the above process, the temporal evolution of the vorticity, temperature, and heat-release distributions within one cycle of the 1T mode of acoustic oscillation is plotted, as shown in Fig. 6-15. The vortex shedding process is clearly visualized in the evolution of the vortex spiral, which gyrates around the chamber centerline and propagates downstream. The wave-like structure on the flame surface possesses a characteristic frequency corresponding to the 1T acoustic wave. Because the vortex shedding affects the shapes of the flame front, it also changes the heat-release distribution. As a result, the acoustic motion in the chamber is closely coupled with the heat-release fluctuation.

### 6.3.2.5 Coupling between Acoustic and Heat-Release Oscillations

The mutual coupling between heat release and acoustic motions can be characterized using the Rayleigh parameter (Rayleigh, 1945), $Ra(x)$, defined as the time-averaged product of the pressure oscillation $p'(x,t)$ and heat-release fluctuation $q'(x,t)$.

$$Ra(x) = \frac{1}{\tau} \int p'(x,t)q'(x,t) \, dt$$ \hspace{1cm} (6.2)

where $\tau$ is the time period of oscillation. The Rayleigh parameter provides a qualitative measure of the extent to which unsteady heat release drives or suppresses instabilities. The acoustic oscillation is amplified if $Ra(x) > 0$, or damped out if $Ra(x) < 0$. Fig. 6-16 presents the spatial distributions of the normalized Rayleigh parameter and the mean flame position (denoted by the black line) on the $x-r$ and $r-\theta$ planes, respectively. A well organized distribution of the
Rayleigh parameter is observed, with four asymmetrical dipoles (i.e., combinations of monopoles and dipoles) located near the edge of the backward-facing step and one near the edge of the center body. These dipoles, with larger positive values on the burnt side of the flame and smaller negative values on the unburnt side, arise from the wave-like distribution of heat release shown in Fig. 6-15. They are closely related to the local vortical motions. The formation of these dipoles can be explained by considering the interaction between the flame and the local acoustic field. During the pressure build-up stage with a positive pressure fluctuation, the flame zone is expanded. The flame front moves into the burnt region and results in a positive heat-release fluctuation on the burnt side and a negative heat-release fluctuation on the unburnt side. In the subsequent stage with a negative pressure fluctuation, the flame zone is reduced. The flame front propagates upstream into the unburnt region and produces a negative heat-release fluctuation on the burnt side and a positive heat-release on the unburnt side. In both stages, the heat-release fluctuation is in phase with the pressure oscillation in the burnt region and results in a positive $Ra(x)$; however, the situation is reversed in the unburnt region and consequently results in a negative $Ra(x)$.

In general, the Rayleigh parameter has a positive value in much of the volume in the flame zone. The acoustic field is favorably correlated with the unsteady heat release and extracts energy from combustion. The chamber exhibits a wide range of oscillation frequencies corresponding to the natural acoustic modes in various parts of the system. The matching of certain acoustic modes and shear-layer instability dominates the process of vortex shedding, and consequently leads to periodic oscillations of the flame front and the ensuing heat-release fluctuations. The distribution of the Rayleigh parameter reflects the coupling between heat release and acoustic waves. When such a feedback-loop process is established, as shown in Fig. 6-17, energy from combustion is fed to the acoustic field and strong instabilities take place in the chamber.
6.3.3 Effect of Inlet Swirl Number on Flame Dynamics

The effects of inlet swirl number on flame dynamics were also studied. Three generic swirlers with swirl angles of $30^\circ$, $45^\circ$ and $55^\circ$ were investigated. The corresponding swirl numbers were 0.44, 0.76 and 1.10, respectively.

Fig. 6-19 shows the mean temperature fields and streamline patterns of these three cases. Three distinct recirculation zones are observed at low swirl number $S = 0.44$: a separation wake recirculation zone (WRZ) behind the centerbody, a CRZ due to the sudden enlargement of the combustor configuration at the dump plane and a CTRZ due to vortex breakdown. However, only CRZ and CTRZ are observed at higher swirl numbers. The inlet swirl number has significant effect on the flow development in the combustion chamber. When there is no swirl, only WRZ and CRZ exist. When the inlet swirl number increases from zero and exceeds a critical value, a vortex breakdown induced recirculation zone is established in the downstream region. As the inlet swirl number further increases, the CTRZ moves upstream and merges with the wake recirculation zone. As a result, a bottleneck-like shape in the recirculation pattern is formed. With the inlet swirl number further increases, the CTRZ continues moving upstream and eventually overrides the WRZ and WRZ disappears, dictating the overall flow development in the chamber. Similar results from experimental work were also reported in Chao (1988).

The mean temperature field in both cases shown in Fig. 6-19 clearly exhibits a double-surface envelope flames anchored at the edges of the center body and the backward-facing step. Flame length is much shorter at low swirl number, which is due to the increased turbulent intensity, as we will show later, and the resultant increased turbulent flame speed and much fast

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* For the cases of $S = 0.44$ and $S = 1.10$, a central-square grid system (see Fig. 6.18) with 3.44 million grid points is used. For the central-square grid system, there is no need to specify boundary conditions at the central singular points, which is different from a 3D axi-symmetric grid system (used for case $S = 0.76$). Also, the physical time step $\Delta t$ for the central-square grid system is larger than that of axi-symmetric grid system (2.5 times in the current cases), which means the overall computation time could be reduced.
fuel consumption rate. Fig. 6-20 presents the snapshots of the temperature field on the \( x-r \) plane at different inlet swirl numbers. Flame flashback phenomena, which are not found at low swirl numbers, are observed at \( S = 1.10 \). The occurrence of flashback is usually attributed to two mechanisms. The first involves flame propagation in the boundary layer along a solid wall where the local velocity diminishes toward the surface. The second mechanism is associated with flow reversal, which is usually caused by vortical motions or acoustics oscillations. In the current case, the flashback is closely linked to the center reverse flow. The reverse flow is so strong at \( S = 1.10 \) that sometimes it can enter into the inlet annulus. As a result, flame anchored by center recirculation zone is convected upstream and flashback occurs.

Fig. 6-21 shows snapshots of the iso-vorticity surface at \( \omega = 75000 \) 1/s (the flow field of \( r > 0.02 \) m is blanked). Spiral vortex structures, which shed from the backward-facing step, are observed in all three cases after the flowfields reach stationary states. The prevalence of spiral vortex at stationary states in all three cases is due to the existence of 1T mode in the chamber, as we will show later. The flame surface is contorted and convoluted by these vortex structures, thus revealing the interactions between the local flow evolution and flame dynamics. The spreading angle of these vortex structures increases with inlet swirl number. Fig. 6-22 shows snapshots of the iso-vorticity surface at \( \omega = 75000 \) 1/s (the flow field of \( r > 0.01 \) m is blanked). A bubble like structure is observed in the downstream \( S = 0.44 \). As the swirl number increase, it moves upstream and collides with the center body. Spiral vortex structure, which shed from the central body can also be found at \( S = 0.44 \). However, at higher swirl numbers, this spiral vortex structure is absorbed by the bubble like structure and disappears, when the bubble like structure approaches the center body.

Fig. 6-23 shows the power spectral densities of pressure fluctuations at three different swirl number. At \( S = 0.44 \), 1L, 1T and 1R modes locate at 1761, 10367 and 22157 Hz, respectively. At \( S = 0.76 \), 1L, 1T and 1R modes locate at 1795, 10970 and 21742 Hz,
respectively. At $S = 1.10$, no 1L mode is found and 1T and 1R modes locate at 10795 and 21872 Hz. The acoustic frequencies observed in the chamber only slightly vary with inlet swirl number, as shown in Fig. 6-23, although their amplitudes are much different. The amplitude of 1L mode decreases with inlet swirl number and disappears at very high inlet swirl number, which may be due to the shrinking of flame surface and reduction of heat release fluctuations near the chamber head-end (i.e., 1L anti-node point).

The heat release and flame surface responses to flow oscillations are very important to understand flame and flow interactions. The total heat release can be obtained as:

$$\dot{Q} = \rho_u \Delta h_f^0 S_f A,$$

where $\rho_u$ is unburnt gas density. $S_f$ is subgrid turbulent flame speed. $\Delta h_f^0$ is heat of reaction and $A$ is total filtered flame surface area. The total filtered flame surface area is integrated as:

$$A = \int \delta(\tilde{G}(\mathbf{x})) |\nabla \tilde{G}(\mathbf{x})| d\mathbf{x} \quad (6.3)$$

where $\delta$ is a delta function, which needs to be evaluated numerically. Note that in level-set flamelet library approaches, $\tilde{G} = 0$ represents the filtered flame front and $\tilde{G}$ has been reinitialized as a signed distance function with $|\nabla \tilde{G}| = 1$. Then, $\delta(\tilde{G}) = 0$ almost everywhere except on the lower dimensional interface (flame surface), which has measure zero. A first order accurate smeared out function of delta function is usually used (Fedkiw, et al., 2003):

$$\delta(\tilde{G}) = \begin{cases} 
1 + \cos(\pi \tilde{G} / \varepsilon) / 2\varepsilon & |\tilde{G}| < \varepsilon \\
0 & |\tilde{G}| > \varepsilon
\end{cases}$$

where $\varepsilon$ is a tunable parameter that determines the size of the bandwidth of numerical smearing. A typically good value is $\varepsilon = 1.5 \Delta$, $\Delta$ is the filter width. This method is widely used to evaluate the quantities defined on arbitrary interfaces in the areas of computer vision and image processing. (Fedkiw, et al., 2003)
Fig. 6-24 shows the power spectral densities of total filtered flame surface area and heat release fluctuations at two different swirl numbers. At $S = 0.44$, there is a dominant mode at 1761 $Hz$, which corresponds to the 1L mode of the combustor. Also a harmonic mode at 3320 $Hz$ is found, which is approximately two times of the frequency of 1L mode. However, the 1T and 1R mode observed in the combustor has little effect on flame surface oscillations. At $S = 1.10$, a small peak (11712 $Hz$) near the 1T mode is observed, which means that the effect of 1T mode oscillation on the flame oscillations is limited. Note that there is no 1L mode exists in the combustor and the dominant one is 1T mode at $S = 1.10$. From the above observations, one can conclude that low-frequency flow perturbations exert a strong influence on the global behavior of the flame, such as total flame surface area variations and heat release fluctuations. High-frequency acoustic oscillations pass through the flame without affecting the global flame behavior significantly. This kind of results agrees well with the analytical model of flame surface and heat release response developed for turbulent flames in Chapter 7.
Fig. 6-1: Computational domain.

Fig. 6-2: Schematic of grid system, total grid points, 176x141x81 = 2.01 million. (the presented grid has fewer points than these used in the calculations, but the distributions of grid points are similar)
Fig. 6-3: Velocity disturbances generated by a Gaussian random number generator
Fig. 6-4: Frequency spectra of turbulent kinetic energy at three different locations along inlet axis

Fig. 6-5: Mean temperature field and streamline pattern
Fig. 6-6: Radial distributions of mean velocity components, pressure and turbulent kinetic energy at various axial locations.
Fig. 6-7: Snapshot of vorticity magnitude field on $x-r$ and $r-\theta$ planes at $t=12.34\ ms$
Fig. 6-8: Snapshot of iso-vorticity surface at $\omega = 75000 \, s^{-1}$ at $t = 12.34 \, ms$ (top: $r > 0.02 \, m$ is blanked; bottom: $r > 0.01 \, m$ is blanked).
Fig. 6-9: 10 Instantaneous streamlines on $r - \theta$ plane at three different locations at $t = 11.91 \text{ ms}$ and $t = 12.34 \text{ ms}$
Fig. 6-10: Power spectral densities of pressure fluctuations at two different locations and spatial distributions of 1T and 1R modes of acoustic oscillation
Fig. 6-11: Temporal evolution of temperature field on \( x - r \) and \( r - \theta \) planes (\( x = 39.2 \text{ mm} \)) over one cycle of 1L mode of oscillation
$x = 0.035 \text{ m}$

Fig. 6-12: Superposition of instantaneous flame surfaces at successive time intervals on $x - r$ and $r - \theta$ planes ($x = 35 \text{ mm}$)
Fig. 6-13: Temporal evolution of iso-thermal surface at $T = 1700\ K$ over one cycle of 1L mode of oscillation
Fig. 6-14: Vortex and flame front interaction over one cycle of 1T mode of oscillation.
Fig. 6-15: Temporal evolution of iso-vorticity surface at $\omega = 75000 \text{ s}^{-1}$ ($r > 0.02 \text{ m}$ is blanked), iso-thermal surface at $T = 1700 \text{ K}$ and normalized heat release contour over one cycle of 1T mode of oscillation.
Fig. 6-16: Distributions of normalized Rayleigh parameter on $x-r$ and $r-\theta$ planes.
Fig. 6-17: Feedback closed loop between combustion dynamics and chamber dynamics
Fig. 6-18: Schematic of central-square grid system, total grid points is 3.44 million (the presented grid has fewer points than these used in the calculations, but the distributions of grid points are similar).
Fig. 6-19: Effects of inlet swirl number on mean temperature field and streamline pattern
Fig. 6-20: Snapshots of temperature fields on $x - r$ plane at three different inlet swirl numbers
Fig. 6-21: Snapshots of iso-vorticity surface at $\omega = 75000 \text{ s}^{-1}$ ($r > 0.02 \text{ m}$ is blanked) at three different inlet swirl numbers
Fig. 6-22: Snapshots of iso-vorticity surface at $\omega = 75000 \, s^{-1}$ ($r > 0.01 \, m$ is blanked) at three different inlet swirl numbers.
Fig. 6-23: Power spectral densities of pressure fluctuations at inlet annulus exit at three different inlet swirl numbers.
Fig. 6-24: Power spectral densities of total flame surface and heat release fluctuations at two different swirl numbers.
Chapter 7

A Kinematic Theory of Premixed Turbulent Flame Response to Flow Oscillations

7.1 Introduction

Under most conditions for premixed flame in practical systems, chemical reaction is confined in a thin, sheet-like laminar flame structure whose inner layer is unaffected by the smallest turbulent eddies (Peters, 2000; Hawkes, 2001), so that a level-set equation can be used to describe the movement of the flame front. One complicating feature of the topology of a flame surface in turbulent flow is that turbulent eddies can wrinkle the flame front or even quench it, while the motions of the flame front modify the flow characteristics. The situation is further complicated due to the existence of coherent structures in many practical turbulent flow fields. The complex coupling between periodic motions and the flame front in turbulent flow field plays an important role in the unsteady behavior of many premixed combustion systems. Understanding such issues and developing the control capabilities is essential for improving combustion efficiency and reducing pollutant emissions. Much of the understanding of coupling between coherent structures and flames stems from the study of flame-vortex interaction (Renard et al., 2000). The vortex can wrinkle and stretch the flame front, which may enhance the flame propagation or lead to flame extinction. The effects of coherent structures on propagation of premixed flames were investigated by Ulitsky and Collins (1997). Their results indicated the flame speed is increased due to the present of coherent structures.

In this chapter, the triple decomposition technique along with level-set equation is used to study the behavior of a turbulent premixed flame under the effects of periodic motions. Emphasis
is placed on the effects of periodic motions on turbulent flame velocity and turbulent flame thickness. Then, a kinematic turbulent flame response model to flow oscillations was developed for a stabilized flame based on the dynamics equation for periodic flame surface motions.

7.2 Dynamical Equations for Mean, Deterministic and Turbulent Motions for Turbulent Premixed Flame

Starting from level-set equation governing the flame front evolution:

$$\frac{\partial G}{\partial t} + u_j \frac{\partial G}{\partial x_j} = S_L \nabla G$$  \hspace{1cm} (7.1)

Triple decomposition gives:

$$u_i = \bar{u}_i + u_i'' + u_i'$$
$$G = \bar{G} + G^a + G'$$  \hspace{1cm} (7.2)

Substituting Eq. 7.2 into Eq. 7.1, taking the time average, and making use of continuity equation, we obtain the equation for $\bar{G}$:

$$\frac{\partial \bar{G}}{\partial t} + \bar{u}_j \frac{\partial \bar{G}}{\partial x_j} = S_L \nabla \bar{G} - \frac{\partial u''_j G^a}{\partial x_j} - \frac{\partial u'_j G'}{\partial x_j}$$  \hspace{1cm} (7.3)

The equation for $G^a$ can be obtained by taking the ensemble phase average of Eq. 7.1 and subtracting Eq. 7.3:

$$\frac{\partial G^a}{\partial t} + \bar{u}_j \frac{\partial G^a}{\partial x_j} + u''_j \frac{\partial G^a}{\partial x_j} = - \frac{\partial u''_j \bar{G}}{\partial x_j} + \frac{\partial u''_j G^a}{\partial x_j} - \frac{\partial (u'_j G')^a}{\partial x_j}$$
$$+ < S_L \nabla G > - S_L \nabla \bar{G}$$  \hspace{1cm} (7.4)
The equation for $G'$ is derived by subtracting the ensemble phase averaged Eq. 7.1 from itself:

$$\frac{\partial G'}{\partial t} + \bar{u}_j \frac{\partial G'}{\partial x_j} + u'_j \frac{\partial G'}{\partial x_j} = - \bar{u}'_j \bar{G} - \frac{\partial u'_j G^a}{\partial x_j} - \frac{\partial}{\partial x_j} (u'_j G' - < u'_j G' >)$$  

$$S_L \nabla |G| > - < S_L |\nabla G| >$$ (7.5)

Similar to momentum equations, three parts of the nonlinear term $-u'_j G'$, which are $-u'_j G'$, $-(u'_j G')^a$ and $-(u'_j G')'$, can be found in mean, periodic and turbulent equations. The eddy viscosity model also can be used to model the term $-u'_j G'$.

$$-u'_j G' = v_i \frac{\partial G}{\partial x_j}$$ (7.6)

However, the above modeling leads to an elliptic equation for $G$, which is inconsistent with the mathematical character of $G$ equation (Peters, 2000). Besides, when Eq. 7.6 is applied,

$$\frac{\partial}{\partial x_j} (-u'_j G') = \frac{\partial}{\partial x_j} (v_i \frac{\partial G}{\partial x_j}) = -v_i \bar{k} |\nabla G| + \bar{n}_j \frac{\partial}{\partial x_j} (v_i \bar{n}_k \frac{\partial G}{\partial x_k})$$ (7.7)

where $\bar{k} = \nabla \cdot \bar{n}$. The last term on the right-hand side of Eq. 7.7 is normal to the flame surface. Its effects can be or already are contained in the modeling turbulent flame speed $S_T$. When the last term of Eq. 7.7 is neglected, the modeling of $-u'_j G'$ becomes:

$$-u'_j G' = v_i \bar{k} |\nabla G| = v_i \bar{k} \frac{\nabla G}{|\nabla G|} \nabla G$$ (7.8)

For modeling of $-(u'_j G')^a$, a similar approach can be used, that leads to:

$$-(u'_j G')^a = v_i \bar{k} \frac{\nabla G}{|\nabla G|} \nabla G^a$$ (7.9)
Depending on the phase difference between $u^a_j$ and $G^a$, $\bar{u}^a_j G^a$ can be expressed as:

$$\bar{u}^a_j G^a = \frac{1}{2} |u^a_j(x)G^a(x)| \cos \phi$$  \hspace{1cm} (7.10)

### 7.3 Turbulence Flame Speed under the Effect of Periodic Motions and Turbulent Motions

In Eq. 7.3, the term $\bar{S_L} \nabla G$ is the flame propagation term. A turbulent flame speed $S_T$ is usually introduced to model this term, which leads to:

$$\bar{S_L} \nabla G = S_T \nabla G = S_T (-\bar{\mathbf{u}} \cdot \nabla G)$$  \hspace{1cm} (7.11)

where $S_T$ is turbulent flame speed and $\bar{\mathbf{u}} = -\nabla G |\nabla G|$. Due to their fundamental importance for premixed combustion theory, turbulent flame speed and flame thickness have been subjects of a large number of theory and experimental investigations for many decades. Damköhler (1940) was the first to present theoretical expressions for the turbulent flame speed. Damköhler expressed the mass flux $\dot{m}$ in terms of turbulent flame speed $S_T$ and surface area of mean flame location $\overline{A}$.

$$\dot{m} = \rho_u S_L A = \rho_u S_T \overline{A}$$  \hspace{1cm} (7.12)

where $\rho_u$ is the density of unburnt mixture and $A$ is the area of instantaneous flame surface location. This leads to:

$$S_T = S_L \frac{A}{\overline{A}} = S_L (1 + \frac{A'}{A})$$  \hspace{1cm} (7.13)
where \( A' \) is the flame surface area fluctuation, which may or may not include the effects of periodic motions. Assuming that the flame surface fluctuation \( A' \) is proportional to the turbulent velocity \( v' \), Damkohler proposed the following model for turbulent flame speed:

\[
S_T = S_L (1 + \frac{v'}{S_L})
\]  

(7.14)

A remark should be made here. The \( S_T \) defined in Eq. 7.13, mathematically, is not exactly the same as \( S_T \) defined in Eq. 7.11 (although they might be equal to each other in some specific cases). However, assuming constant \( S_L \) and using Reynolds decomposition, we obtain:

\[
S_T = \frac{1}{-\bar{n} \cdot \nabla G} \frac{S_L}{\partial x_j} (-n_j) \frac{\partial G}{\partial x_j}
\]

\[= S_L (1 + \frac{1}{\bar{n} \cdot \nabla G} n_j' \frac{\partial G'}{\partial x_j})
\]

(7.15)

As we can see, Eq. 7.15 and Eq. 7.14 are similar in that both contain the laminar flame speed term and the fluctuation term due to turbulent motions, which means that their modeling is similar and might be able to replace each other. Many models have been proposed to modify Damkohler’s analysis for turbulent flame speed, most of which take the following form:

\[
S_T = S_L (1 + C (\frac{v'}{S_L})^n)
\]

(7.16)

where \( C \) and \( n \) are two constants that need to be specified. Lipatnikow and Chomiak (2002), in their recent review, performed a survey of research work on the study of turbulent flame speed. Several qualitative trends are obtained, such as an increase in \( S_T \) with turbulent velocity \( v' \); an increase in \( S_T \) and by \( S_L \) with scaling exponent \( n \) being close to 0.5/0.8; and an increase in \( S_T \) by pressure despite the decrease in \( S_L \).
However, few of models for turbulent flame speed $S_T$ takes into account the effects of periodic motion, although some work (Ulitsky and Collins, 1997) has been done to investigate the effects of coherent structure on turbulent flame speed. To account for the effects of periodic motion, we use the triple decomposition techniques introduced above:

$$n_j = \overline{n}_j + n_j^a + n_j^f$$

$$S_L = \overline{S}_L + S_L^a$$ \hspace{1cm} (7.17)

Note that even though a flamelet assumption is made, which means that flame inner structure is unaffected by the smallest scale turbulence, the interaction of flow/flame will change flow field and subsequently modify the incoming fresh gas property (such as equivalence ratio, etc.) before it reaches the flame, thus inducing periodic change in the laminar flame speed. Then, $S_T$ can be written as:

$$S_T = \frac{1}{\overline{n} \cdot \nabla G} \frac{\partial \overline{G}}{\partial \overline{x}_j} = \frac{1}{\overline{n} \cdot \nabla G} \overline{S}_L (-n_j) \frac{\partial G}{\partial \overline{x}_j}$$

$$S_T = \overline{S}_L (1 + \frac{1}{\overline{n} \cdot \nabla G} n_j^a \frac{\partial G^a}{\partial x_j} + \frac{1}{\overline{n} \cdot \nabla G} n_j^f \frac{\partial G^f}{\partial x_j} + \frac{1}{\overline{n} \cdot \nabla G} S_L^a n_j \frac{\partial G}{\partial \overline{x}_j}) \hspace{1cm} (7.18)$$

As we can see, there are four terms in the expression for turbulent flame speed $S_T$. The first term is mean laminar flame speed. The second term represents the effects of periodic motions on turbulent flame speed. The third term represents the effects of turbulent motions on turbulent flame speed. The last term is due to the change of laminar flame speed itself. The last four terms need to be taken into account separately to model the turbulent flame speed. By analogy, in modeling Eq. 7.16, a simple model is proposed as follows:

$$S_T = S_L (1 + C_1 (\frac{v^a}{S_L})^m + C_2 (\frac{v^f}{S_L})^n) \hspace{1cm} (7.19)$$
where $C_1, C_2, m$ and $n$ are constants that need to be specified. In Eq. 7.4 the term

\[ (S_L |\nabla G|) = (S_L |\nabla G|^3) \]  

also needs to be modeled. Similarly, another flame speed $S_A$, which can be called acoustic flame speed, can be introduced for modeling purpose.

\[ (S_L |\nabla G|^a) = S_A(-\mathbf{n} \cdot \nabla G^a) = S_A\left(\frac{\nabla G^a}{\nabla G}\right) \]  

(7.20)

Using triple decomposition

\[
S_A = \frac{(S_L |\nabla G|^a)}{(-\mathbf{n} \cdot \nabla G^a)} = \frac{< S_L (-n_j) \partial G / \partial x_j > - S_L (-n_j) \partial G / \partial x_j}{(-\mathbf{n} \cdot \nabla G^a)}
\]

\[
= S_L \left(1 + \frac{n_j^2 \partial G / \partial x_j}{\mathbf{n} \cdot \nabla G^a} + \frac{(n_j \partial G^a / \partial x_j)^a}{\mathbf{n} \cdot \nabla G^a} + \frac{(n_j' \partial G^a / \partial x_j)^a}{\mathbf{n} \cdot \nabla G^a} - S_L n_j \partial G / \partial x_j)^a}{\mathbf{n} \cdot \nabla G^a} \right) \]  

(7.21)

Although there are five terms in the expression for acoustic flame speed $S_A$, it is very similar to the expression for $S_T$. The first term is mean laminar flame speed. The second term reflects the interaction between periodic and mean motion. The third term represents the effects of periodic motion on acoustic flame speed. The fourth term represents the effects of turbulent motion on acoustic flame speed. The last term is due to the change in laminar flame speed itself. The effects of the last four terms need to be included in the modeling of $S_A$. For the sake of simplicity, we just assume that the modeling of $S_A$ is the same as that for $S_T$.

### 7.4 Turbulence Flame Thickness under the Effect of Periodic Motions and Turbulent Motions

The turbulent flame thickness $l_{F,t}$ can be defined as:
where \( G' = G^a + G' \), and \( \overline{G'^2} \) is flame surface fluctuation under the effects of both periodic motion and turbulent motions.

\[
\overline{G'^2} = (G^a + G')(G^a + G')
\]

\[
= (G^a)^2 + (G')^2
\]  

Eq. 7.23 states that the turbulent flame surface fluctuation can be divided into two parts: the flame surface fluctuation due to periodic motion and flame surface fluctuation resulting from background turbulent motion.

The equation for \( (\overline{G^a})^2 \) can be obtained after multiplying Eq. 7.4 by \( 2G^a \) and taking the time average:

\[
\frac{\partial (\overline{G^a})^2}{\partial t} + \bar{u}_j \frac{\partial (\overline{G^a})^2}{\partial x_j} + u_j^a \frac{\partial (\overline{G^a})^2}{\partial x_j} = -G^a u_j^a \frac{\partial \overline{G^a}}{\partial x_j} + 2(u_j' G')^a \frac{\partial G^a}{\partial x_j}
\]

\[
- \frac{\partial}{\partial x_j} (2G^a(u_j' G')^a) + 2G^a (<S_L|\nabla G|> - S_L|\nabla G|)
\]

The equation for \( (\overline{G'})^2 \) can be obtained after multiplying Eq. 7.5 by \( 2G' \) and taking the time average:

\[
\frac{\partial (\overline{G'})^2}{\partial t} + \bar{u}_j \frac{\partial (\overline{G'})^2}{\partial x_j} + u_j' \frac{\partial (\overline{G'})^2}{\partial x_j} = -2u_j' G' \frac{\partial \overline{G'}}{\partial x_j} - 2(u_j' G')^a \frac{\partial G^a}{\partial x_j} - 2(u_j' G')^a \frac{\partial G^a}{\partial x_j}
\]

\[
- \frac{\partial}{\partial x_j} 2G' (u_j' G')^a + 2(u_j' G') ^a \frac{\partial G^a}{\partial x_j} + 2G' (S_L|\nabla G| - <S_L|\nabla G|>)
\]
As we can see, the two terms $\overline{(G^a)^2}$ and $\overline{(G^t)^2}$ are not really decoupled from each other. Their interactions are characterized by the term, $2(u'_i G^a) \frac{\partial G^a}{\partial x_j}$, which appears in both Eq. 7.24 and Eq. 7.25, but with opposite signs.

### 7.5 Modeling of Heat Release Response to Flow Oscillations

In this section, the flame surface equations obtained in the previous sections are used to derive a turbulent flame heat release response model to flow oscillation for the stabilized flame in a model combustor. The model combustor of concern consists of a single-swirl injector, an axisymmetric chamber, and a choked nozzle. Experimental study (Broda et al., 1998; Seo, 1999) and our previous numerical study have been performed to investigate the flame dynamics in this combustor. The mean temperature contour and streamlines for the stable flame and unstable flame (inlet swirl number at 0.76) in the combustor are shown in Fig. 5-8 and Fig. 6-5.

The mixture consumption rate $\dot{m}$ can be expressed as

$$\dot{m} = \rho_u S_L \bar{A} = \rho_u S_{T,a} < A > = \rho_u S_T \bar{A}$$

(7.26)

The turbulent flame speed $S_T$ is introduced here according to area of long time-averaged flame surface location, $\bar{A}$. The turbulent flame speed $S_{T,a}$ corresponds to the area of ensemble-averaged flame surface location for a particular phase, $< A >$, which can be further expressed as $< A > = \bar{A} + A^\prime$. Note that $S_T$ represents an acoustic enhanced turbulent flame speed, which includes the effects of periodic flame surface motions, while $S_{T,a}$ only includes the effects of background turbulent motions. The heat release $\dot{Q}$ $(J/s)$ is given by
Application of the triple decomposition to Eq. 7.27 and linearization of the result yields the long time-averaged and fluctuating heat release as shown below.

\[
\dot{Q} = \rho_u S_L A q = \rho_u S_{T,a} < A > q = \rho_u S_T \bar{A} q
\]  

(7.27)

Divide Eq. 7.29 by Eq. 7.28 to yield:

\[
\hat{Q} = \bar{\rho}_u \bar{S}_{T,a} \bar{A} \bar{q}
\]  

(7.28)

\[
\hat{Q}^a = \bar{\rho}_u \bar{S}_{T,a} \bar{A} q^a + \bar{\rho}_u S_{T,a} A \bar{q} + \bar{\rho}_u S_{T,a} \bar{A} \bar{q} + \bar{\rho}_u \bar{S}_{T,a} A^a \bar{q}
\]  

(7.29)

Divide Eq. 7.29 by Eq. 7.28 to yield:

\[
\frac{\dot{Q}^a}{\bar{Q}} = \frac{q^a}{\bar{q}} + \frac{\rho_u^a}{\bar{\rho}_u} + \frac{S_{T,a}^a}{\bar{S}_{T,a}} + \frac{A^a}{\bar{A}}
\]  

(7.30)

Note that the oscillations of turbulent flame speed \( S_{T,a} \) (only including the effects of background turbulent motions) mainly come from the oscillations of laminar flame speed \( S_L \), as a result, \( S_{T,a}^a / \bar{S}_{T,a}^a \approx S_L^a / \bar{S}_L \). Then there are four sources contributing to the heat release oscillations: heat of reaction, density, laminar flame speed, and flame surface area.

In the present study, we focus on the behavior of unsteady heat release fluctuations due to the flame surface fluctuations and neglect the other source of fluctuations. Then the heat release oscillations due to periodic flame surface motions can be expressed as:

\[
\frac{\dot{Q}^a}{\bar{Q}} = \frac{A^a}{\bar{A}}
\]  

(7.31)

To obtain the flame surface variation, we start from the modeled dynamical equation for mean and periodic flame surface motions:
Assume that flowfield and flame are axi-symmetric and the curvature effects on turbulent flame speed are neglected. In a cylindrical coordinate system, the above two equations can be linearized as:

$$\frac{\partial G}{\partial t} + \bar{u}_r \frac{\partial G}{\partial r} + \bar{u}_z \frac{\partial G}{\partial z} = S_T \sqrt{V_G}$$  \hspace{1cm} (7.34)

$$\frac{\partial G_a}{\partial t} + \bar{u}_r \frac{\partial G_a}{\partial r} + \bar{u}_z \frac{\partial G_a}{\partial z} = S_T \sqrt{V_G} \frac{\nabla G_a}{\nabla G}$$  \hspace{1cm} (7.35)

Replacing $G(x,r,t)$ by $x - \xi(r,t)$, where $\xi(r,t)$ is the axial displacement of the flame surface, we obtain:

$$G(x,r,t) = x - \xi(r,t)$$  \hspace{1cm} (7.36)

$$G^a(x,r,t) = -\xi^a(r,t)$$  \hspace{1cm} (7.37)

Substituting Eq. 7.36 and Eq. 7.37 into Eq. 7.34 and Eq. 7.35, we obtain:

$$-\bar{u}_r \frac{d\xi}{dr} + \bar{u}_z = S_T \sqrt{\left(\frac{d\xi}{dr}\right)^2 + 1}$$  \hspace{1cm} (7.38)

$$-\frac{\partial \xi^a}{\partial t} - \bar{u}_r \frac{\partial \xi^a}{\partial r} - u_r \frac{\partial \xi}{\partial r} + u_z = S_T \frac{d\xi}{dr} \sqrt{\left(\frac{d\xi}{dr}\right)^2 + 1} \frac{\partial \xi^a}{\partial r}$$  \hspace{1cm} (7.39)
The above equations will be applied to study the turbulent flame response in both stable and unstable flame. The stable flame, which is anchored by central recirculation zone alone, will be considered first. For illustrative purposes, a schematic of the stable flame is shown in Fig. 7-1.

The initial and boundary conditions for Eq. 7.39 for stable flame are:

$$\xi^a(r,0) = 0 \quad \text{and} \quad \xi^a(r_t, t) = 0 \quad (7.40)$$

Let $\xi^a = \xi^a e^{i\alpha \theta}$, $u^a_x = \hat{u}^a_x e^{i\alpha \theta}$, $u^a_r = \hat{u}^a_r e^{i\alpha \theta}$ and substitute them into Eq. 7.39:

$$i\omega \hat{\xi}^a = - (\bar{u}_r + S_T) \frac{d \bar{\xi}}{dr} / \sqrt{\left( \frac{d \bar{\xi}}{dr} \right)^2 + 1} \frac{d \hat{\xi}}{dr} - \hat{u}^a_r \frac{\partial \bar{\xi}}{\partial r} + \hat{u}^a_x \quad (7.41)$$

Assuming that $\bar{u}_x$ and $\bar{u}_r$ are independent of $r$ and using boundary condition: $\hat{\xi}(r_t) = 0$, from Eq. 7.41 we obtain:

$$\hat{\xi}^a(r) = n \frac{i \omega}{i \omega} (1 - e^{m(r-r)}) \quad (7.42)$$

where $m = \bar{u}_r + S_T \frac{d \bar{\xi}}{dr} / \sqrt{(d \bar{\xi}/dr)^2 + 1}$, $n = \hat{u}^a_x - \hat{u}^a_r \frac{d \bar{\xi}}{dr}$.

The instantaneous flame surface area can be calculated by integral

$$A = \int_{\chi}^{\chi} 2\pi r \sqrt{1 + \left( \frac{\partial \bar{\xi}}{\partial r} \right)^2} \, dr \quad (7.43)$$

Using the Taylor series, $f(x) = f(x_0) + f'(x_0)(x-x_0) + f''(x_0) \frac{(x-x_0)^2}{2} + \ldots$. Eq. 7.43 can be rewritten as:

$$A = \int_{\chi}^{\chi} 2\pi r \sqrt{1 + \left( \frac{\partial \bar{\xi}}{\partial r} \right)^2} \, dr = \int_{\chi}^{\chi} 2\pi r \sqrt{1 + \left( \frac{\partial \bar{\xi}}{\partial r} \right)^2} + \frac{d \bar{\xi}}{dr} / \sqrt{(d \bar{\xi}/dr)^2 + 1} \, dr + \ldots) \, dr \quad (7.44)$$
Then the mean flame surface area:

\[ \bar{A} = 2\pi \int_{r_1}^r \sqrt{1 + \left( \frac{\partial \xi}{\partial r} \right)^2} \, dr \]  \hspace{1cm} (7.45)

Then flame surface area change due to periodic motions is:

\[ A^a = 2\pi \int_{r_1}^r \frac{d\xi}{dr} \frac{d\xi^a}{dr} \frac{d\xi^a}{dr} \]  \hspace{1cm} (7.46)

Assume that \( d\xi / dr \) is independent of \( r \). Then heat release oscillation can be expressed as:

\[
\frac{\dot{Q}^a}{\dot{Q}} = \frac{A^a}{\bar{A}} = \frac{2}{(r_2^2 - r_1^2) \left( (d\xi / dr)^2 + 1 \right)} \left( \int_{r_1}^r \left( \frac{d(\xi^a / r)}{dr} - \frac{\xi^a}{r} \right) dr \right)
\]

\[
= \frac{2}{(r_2^2 - r_1^2) \left( (d\xi / dr)^2 + 1 \right)} \left( \frac{n}{i\omega} r_2 \left( 1 - e^{i\omega(\tau - \tau_0)} \right) - \frac{n}{i\omega} (r_2 - r_1 + \frac{m}{i\omega} (e^{i\omega(\tau - \tau_0)} - 1)) \right)
\]

\[
= \frac{2}{(r_2^2 - r_1^2) \left( (d\xi / dr)^2 + 1 \right)} \left( \frac{n}{i\omega} \left( r_1 + \frac{m}{i\omega} \right) - \left( r_2 + \frac{m}{i\omega} \right) e^{i\omega(\tau - \tau_0)} \right)
\]  \hspace{1cm} (7.47)

The mean \( \bar{u}_z \), \( \bar{u}_x \) and the shape of mean flame front \( \bar{\xi} = \bar{\xi}(r) \) can be extracted from the computational results. \( S_T \) can be obtained either from our previous model, which needs inputting local turbulent velocity, or directly from Eq. 7.38. The latter method is used in the present study to obtain \( S_T \). \( d\xi / dr \approx \tan \alpha \) is assumed for stable flame, as shown in Fig. 7-1., and \( \alpha \) is extracted from the computational result. We define a non-dimensional frequency as \( \Omega = \omega(2 - 1) / m \), then

\[
\frac{\dot{Q}^a}{\dot{Q}} = \frac{\sin 2\alpha}{(r_2 + r_1) m i\Omega} \left( \frac{r_2 - r_1}{i\Omega} - \left( \frac{r_2 - r_1}{i\Omega} \right) e^{-i\Omega} \right)
\]

\[
= R_x \frac{\hat{u}_x^a}{\bar{u}_x} + R_y \frac{\hat{u}_y^a}{\bar{u}_y}
\]  \hspace{1cm} (7.48)
where

\[
\begin{align*}
R_u &= \frac{\bar{u}_x \sin 2\alpha}{i\Omega(r_2 + r_1)(\bar{u}_r + S_T \sin \alpha)} \left( r_1 + \frac{r_2 - r_1}{i\Omega} - \left( r_2 + \frac{r_2 - r_1}{i\Omega} \right) e^{-i\Omega} \right) \\
R_v &= -\frac{2\bar{u}_x \sin^2 \alpha}{i\Omega(r_2 + r_1)(\bar{u}_r + S_T \sin \alpha)} \left( r_1 + \frac{r_2 - r_1}{i\Omega} - \left( r_2 + \frac{r_2 - r_1}{i\Omega} \right) e^{-i\Omega} \right)
\end{align*}
\]  
(7.49)

The amplitude and phase of transfer function coefficients \( R_u \) are:

\[
|R_u| = \frac{\bar{u}_x \sin 2\alpha}{\Omega(r_2 + r_1)(\bar{u}_r + S_T \sin \alpha)} \sqrt{(r_1 - r_2 \cos \Omega + \frac{r_2 - r_1}{\Omega} \sin \Omega)^2 + (r_2 \sin \Omega + (\cos \Omega - 1) \frac{r_2 - r_1}{\Omega})^2}
\]

\[
\text{Phase}(R_u) = \tan^{-1}\left\{ \frac{(r_2 \sin \Omega + (\cos \Omega - 1) \frac{r_2 - r_1}{\Omega})}{(r_1 - r_2 \cos \Omega + \frac{r_2 - r_1}{\Omega} \sin \Omega)} \right\}
\]

Similar results can also be obtained for \( R_v \).

The heat release response model presented by Eq. 7.49 can be verified against the model previously derived by Dowling (1999). In the limiting case where \( \bar{u}_r = 0 \), and utilizing the expression \( S_T = -\bar{u}_r \sin \alpha + \bar{u}_x \cos \alpha \) (from Eq. 7.38), Eq. 7.49 reduces to Dowling’s model:

\[
\begin{align*}
R_u &= \frac{2}{i\Omega(r_2 + r_1)} \left( r_1 + \frac{r_2 - r_1}{i\Omega} - \left( r_2 + \frac{r_2 - r_1}{i\Omega} \right) e^{-i\Omega} \right) \\
R_v &= 0
\end{align*}
\]  
(7.50)

Fig. 7-2 shows the amplitude of the coefficient \( R_u \) as a function of frequency. The amplitude of transfer function coefficient \( R_u \) displays a non-monotonic, decaying sinusoidal behavior, with its highest value near the zero frequency. The high-frequency oscillation passes through the flame without affecting the flame surface area variations and heat release fluctuation significantly. Low frequency perturbations exert a strong influence on the unsteady heat release fluctuations. The results are consistent with the observations of Dowling (1999) and Fleifil et al. (1996). Model Eq. 7.50 and model Eq. 7.49 are also compared. The trends remain the same, but model Eq. 7.50 overestimates the absolute values of amplitude near zero frequency. Fig. 7-3
shows the phase angle of $R_u$ as a function of frequency. A saw blade shape is observed for both models.

Similar methodology described above can be applied to study the unstable flame response. A schematic of the unstable flame is shown in Fig. 7-4. The flame (lower) anchored by the central recirculation zone intersects with the flame (upper) anchored by the corner recirculation zone. The initial and boundary conditions for unstable flame are:

$$\xi^a(r,0) = 0, \quad \xi^a(r_1,t) = 0, \quad \text{and} \quad \xi^a(r_2,t) = 0$$  \hspace{1cm} (7.51)

The mean $\bar{u}_r$, $\bar{u}_x$, $S_r$ and the shape of mean flame front $\bar{\xi} = \bar{\xi}(r)$ can also be extracted from the computational results. It is assumed that $d\bar{\xi}_1/dr \approx \tan \alpha_1$ for the lower flame and $d\bar{\xi}_2/dr \approx \tan \alpha_2$ for the upper flame as shown in Fig. 7-4. The heat release oscillation can be obtained as:

$$\hat{\dot{Q}}^{a} = \frac{\sin 2\alpha_1}{(r_4 + r_1)m_1} \frac{n_1}{i\Omega_1} (r_1 + \frac{r_4 - r_1}{i\Omega_1} - (r_4 + \frac{r_4 - r_1}{i\Omega_1})e^{-i\Omega_1})$$

$$+ \frac{\sin 2\alpha_2}{(r_4 + r_1)m_2} \frac{n_2}{i\Omega_2} (r_3 + \frac{r_4 - r_3}{i\Omega_2} - (r_4 + \frac{r_4 - r_3}{i\Omega_2})e^{-i\Omega_2})$$ \hspace{1cm} (7.52)

$$= R_u \frac{\hat{u}_r^a}{\bar{u}_r} + R_s \frac{\hat{u}_x^a}{\bar{u}_x}$$

where

$$R_u = \frac{\bar{u}_r \sin 2\alpha_1}{i\Omega_1 (r_4 + r_1)(\bar{u}_r + S_r \sin \alpha_1)} (r_1 + \frac{r_4 - r_1}{i\Omega_1} - (r_4 + \frac{r_4 - r_1}{i\Omega_1})e^{-i\Omega_1})$$

$$+ \frac{\bar{u}_r \sin 2\alpha_2}{i\Omega_2 (r_4 + r_1)(\bar{u}_r + S_r \sin \alpha_2)} (r_3 + \frac{r_4 - r_3}{i\Omega_2} - (r_4 + \frac{r_4 - r_3}{i\Omega_2})e^{-i\Omega_2})$$

$$R_s = \frac{2\bar{u}_r \sin^2 \alpha_1}{i\Omega_1 (r_4 + r_1)(\bar{u}_r + S_r \sin \alpha_1)} (r_1 + \frac{r_4 - r_1}{i\Omega_1} - (r_4 + \frac{r_4 - r_1}{i\Omega_1})e^{-i\Omega_1})$$

$$+ \frac{2\bar{u}_r \sin^2 \alpha_2}{i\Omega_2 (r_4 + r_1)(\bar{u}_r + S_r \sin \alpha_2)} (r_3 + \frac{r_4 - r_3}{i\Omega_2} - (r_4 + \frac{r_4 - r_3}{i\Omega_2})e^{-i\Omega_2})$$  \hspace{1cm} (7.53)
and \( m_1 = \bar{u}_r + S_T \frac{d\bar{\xi}_1}{dr} \), \( n_1 = \hat{u}_r^a - \hat{u}_r^a \frac{d\bar{\xi}_1}{dr} \), \( \Omega_1 = \omega(r_4 - r_1) / m_1 \),

\[
m_2 = \bar{u}_r + S_T \frac{d\bar{\xi}_2}{dr} \sqrt{(d\bar{\xi}_2/dr)^2 + 1} \), \( n_2 = \hat{u}_r^a - \hat{u}_r^a \frac{d\bar{\xi}_2}{dr} \), \( \Omega_2 = \omega(r_4 - r_2) / m_2 \)
\]

The amplitude and phase of transfer function \( R_u \) are:

\[
|R_u| = \sqrt{[a_1 (r_1 - r_4 \cos \Omega_1 + \frac{r_4 - r_1}{\Omega_1} \sin \Omega_1) + a_2 (r_3 - r_4 \cos \Omega_2 + \frac{r_4 - r_3}{\Omega_2} \sin \Omega_2)]^2 + [a_1 (r_4 \sin \Omega_1 + (\cos \Omega_1 - 1) \frac{r_4 - r_1}{\Omega_1} \sin \Omega_1) + a_2 (r_4 \sin \Omega_2 + (\cos \Omega_2 - 1) \frac{r_4 - r_3}{\Omega_2} \sin \Omega_2)]^2}
\]

\[
\text{Phase}(R_u) = \tan^{-1} \left\{ \frac{a_1 (r_4 \sin \Omega_1 + (\cos \Omega_1 - 1) \frac{r_4 - r_1}{\Omega_1} \sin \Omega_1) + a_2 (r_4 \sin \Omega_2 + (\cos \Omega_2 - 1) \frac{r_4 - r_3}{\Omega_2} \sin \Omega_2)}{a(r_1 - r_4 \cos \Omega_1 + \frac{r_4 - r_1}{\Omega_1} \sin \Omega_1) + a_2 (r_3 - r_4 \cos \Omega_2 + \frac{r_4 - r_3}{\Omega_2} \sin \Omega_2)} \right\}
\]

where \( a_1 = \frac{\bar{u}_r \sin 2\alpha_1}{\Omega_1 (r_4 + r_1) (\bar{u}_r + S_T \sin \alpha_1)} \) and \( a_2 = \frac{\bar{u}_r \sin 2\alpha_2}{\Omega_2 (r_4 + r_1) (\bar{u}_r + S_T \sin \alpha_2)} \).

Fig. 7-5 and Fig. 7-6 show the amplitude and phase of the coefficient \( R_u \) as a function of frequency. Similar to the stable flame, a non-monotonic, decaying sinusoidal behavior is observed for transfer function coefficient \( R_u \). The high-frequency oscillation passes through the flame without affecting the flame surface area variation and heat release fluctuation significantly. Low frequency perturbations exert a strong influence on the unsteady heat release fluctuation. The combustion responses of stable and unstable flame to flow oscillations are also compared. It seems that the flow oscillations exert a stronger influence on the unsteady heat release fluctuations in unstable flames than in stable flames.
A three-dimensional acoustic analysis was performed by You et al. (2003b) to investigate the stability behavior of the lean-premixed gas-turbine combustor chamber (Broda et al., 1998). In their analysis, a wave equation governing the oscillatory field in the chamber is solved:

\[
\nabla^2 p' - \frac{1}{c^2} \frac{\partial^2 p'}{\partial t^2} = h(\overline{\rho}, \overline{p}, u', p', q', etc.)
\]

subject to boundary condition: \( n \cdot \nabla p' = -f \) (7.54)

Various source terms of unsteady heat release have been taken into account using Eq. 7.27, including the flame surface variations, density variation, flame speed and heat of reaction variations. The combustion chamber is discretized axially into a number of cells such that a combined modal-expansion and spatial-averaging technique can be applied to treat the unsteady motions in the transverse plane of each cell. The oscillatory flow properties are matched at the interface of each pair of adjacent cells by applying the conservation laws to determine the stability characteristics of the entire combustor. The mean flow properties are acquired from numerical calculations. Two cases, which correspond to the stable (\( T_{in} = 600 \text{ K} \)) and unstable (\( T_{in} = 660 \text{ K} \)) operating conditions, are investigated respectively. The solved acoustic frequencies of the first longitudinal mode are close to the experimental value of 1750 Hz. For the stable flame, the damping coefficient is positive, but becomes negative for the unstable flame, which is also consistent with the experiment observations. These results show that the combustion response function derived in the present study can accurately predict the effect of unsteady heat release to a certain extent.
Fig. 7-1: Schematic of the stable flame

Fig. 7-2: The amplitude of $R_u$ as the function of frequency. (stable flame: $r_1 = 4.765 \text{ mm}$, $r_2 = 22.5 \text{ mm}$, $\alpha = 60^\circ$, $\bar{u}_x = 58.0 \text{ m/s}$, Eq. 7.49: $\bar{u}_r = 12.0 \text{ m/s}$, Eq. 7.50: $\bar{u}_r = 0.0 \text{ m/s}$)
Fig. 7-3: The phase angle of $R_u$ as the function of frequency. (stable flame: $r_1 = 4.765 \text{ mm}$, $r_2 = 22.5 \text{ mm}$, $\alpha = 60^\circ$, $\bar{u}_x = 58.0 \text{ m/s}$, Eq. 7.49: $\bar{u}_r = 12.0 \text{ m/s}$, Eq. 7.50: $\bar{u}_r = 0.0 \text{ m/s}$.

Fig. 7-4: Schematic of the unstable flame
Fig. 7-5: The amplitude of $R_u$ as the function of frequency. (unstable flame: $r_1 = 4.765 \text{ mm}$, $r_3 = 10.15 \text{ mm}$, $\alpha_1 = 60^0$, $\alpha_2 = 79^0$, $\overline{u}_x = 85.5 \text{ m/s}$, $\overline{u}_r = 16.3 \text{ m/s}$)

Fig. 7-6: The phase angle of $R_u$ as the function of frequency. (unstable flame: $r_1 = 4.765 \text{ mm}$, $r_3 = 10.15 \text{ mm}$, $\alpha_1 = 60^0$, $\alpha_2 = 79^0$, $\overline{u}_x = 85.5 \text{ m/s}$, $\overline{u}_r = 16.3 \text{ m/s}$)
Chapter 8

Summary and Future Work

8.1 Summary

The research work conducted for this thesis includes a variety of basic and practical issues related to the modeling and simulation of combustion dynamics in gas-turbine engines. In particular, a comprehensive numerical analysis has been established to investigate the combustion dynamics in a swirl-stabilized combustor based on a large-eddy-simulation technique. The flame dynamics and its interactions with turbulence are treated using a level-set flamelet library approach. The model provides a predictive capability for treating premixed turbulent combustion with strong swirling motions, with the acoustic flow properties solved as a part of the results. As a specific example, a lean-premixed system with a single swirl-injector was carefully studied.

The Rayleigh criterion, which has been used in many qualitative descriptions of combustion instabilities, is revisited using a triple decomposition technique. It is found that periodic motions can obtain energy from several sources. They can extract energy from mean flows; they can receive energy from chemical reactions; they can exchange energy with background turbulent motions; they also will be dissipated into thermal energy. When there are no chemical reactions, the major energy source for periodic motions is the mean flow. With combustion, heat release from chemical reactions is the major energy source for driving acoustic motions. The transfer of energy from chemical for chemical reactions only takes place when heat release oscillations are in phase with pressure oscillations. The present study also reveals that
unsteady heat transfer and dissipation play the same role in driving flow oscillations as unsteady heat release.

To model the complex flame evolution in the combustor chamber, a level-set flamelet library approach is developed to simulate premixed turbulent combustion in the context of large eddy simulation. In this model, the flame front is represented by an arbitrary iso-surface $G_0$ in a scale field $G$ whose evolution is formulated using the so-called $G$-equation. Outside the flame front, $G$ is established as a distance function using the re-initialization process. This approach, along with a laminar flamelet library and a presumed PDF method, proves to be a desirable tool for the realistic treatment of premixed turbulent combustion.

The stable flame dynamics and the bifurcation of flame structure from a stable to an unstable state are investigated using two-dimensional axi-symmetric simulation. It was found that the inlet air temperature and equivalence ratio are the two most important variables determining the stability characteristics of the combustor. A slight increase in the inlet airflow temperature across the stability boundary leads to a sudden increase in chamber flow oscillations. One major factor that contributes to this phenomenon is that as the inlet air temperature increases, the flame originally anchored in the center recirculation zone flashes back through the wall boundary layers and the vortical flow downstream of the dump plane. As a result, the flame becomes stabilized by both the corner- and center-recirculating flows. The flame then flaps dynamically and drives flow oscillations through its influence on unsteady heat release. Various fundamental processes such as the high temperature mixture filling process, flame trapping process, and vortex flashback process, responsible for the flame transition from a stable to an unstable state were identified and quantified.

The lean-premixed system operating in an unstable mode was also carefully studied using three-dimensional LES simulation, with emphasis on the unsteady flow/flame structures and the key physical processes responsible for driving combustion instabilities. Good agreement with
analytical solution and experimental observations was obtained in terms of chamber acoustic characteristics and flame shape. The instantaneous flow-field exhibits very complex structures, including the bubble and spiral modes of vortex breakdown and a precessing vortex core (PVC), due to the intrinsic shear layer instability and its coupling with swirling motions. Several physical processes responsible for driving combustion instabilities in the chamber have been identified and quantified, including the mutual coupling between acoustic wave motions, vortex shedding, and flame oscillations. The vortical motions in the flame zone resonate intimately with the acoustic oscillations in the chamber, and give rise to large excursions of unsteady motions. The flame is contorted and convoluted by the local flow oscillations, with the wave number of its surface structure determined by the interactions among the shear- and acoustic-wave instabilities. When such a feedback-loop process is established, energy from combustion is fed to the acoustic field and strong instabilities take place in the chamber. The effects of inlet swirl number on the flow development and flame dynamics in the chamber are also carefully studied.

The last part of the thesis presents a kinematic theory of premixed turbulent flame response to flow oscillations. The triple decomposition technique along with level-set equation is used to study the behavior of turbulent premixed flame under the effects of periodic motions. It was found that the effects of periodic motion have very important effects on turbulent flame speed and turbulent flame thickness. Modeling of these two parameters requires considering the effects of large-scale periodic motions, which are usually geometry dependent. Thus, perhaps there is no universal model for these two parameters. A kinematic turbulent flame response model to flow oscillation was also developed for a stabilized flame based on the dynamics equation for periodic flame surface motions. The resultant model, after being incorporated into a three-dimensional linear acoustic analysis, can accurately predict the effect of unsteady heat release to a certain extent.
8.2 Recommendation for Future Work

In the present numerical study, the focuses have been placed on the roles of hydrodynamic instabilities and flame surface variations on combustion instabilities. The influences of the equivalence ratio on combustion dynamics are isolated using a perfect mixing assumption. However, in practical systems, mixing is usually far from perfect. Experimental measurements (Seo, 1999) indicate that the degree of premixing becomes worse as the injection location approaches the dump plane, since the convection time for mixing becomes shorter. The equivalence ratio oscillation is one of the major sources of heat release fluctuations, and is one of the most important factors determining the characteristics of instabilities. Its effects on combustion dynamics need to be addressed in the future.

In many combustion applications, the fuel and oxidizer enter separately, but are partially mixed by turbulence. Combustion takes place in a stratified medium once the mixture is ignited. Such a mode of combustion has traditionally been called partially premixed combustion (Peters, 2000). This is specifically the case in devices where liquid injection of the fuel is retained, leading to partially premixed flames (gas turbine, diesel engines), which means that investigations of partially premixed flame and spray combustion are necessary.

The level-set flame approach can be used only for premixed combustion. Research work would benefit from an improved turbulent combustion model that can be used to properly treat partially premixed flame and spray combustion. This advanced turbulent combustion model is expected to be able to take care of extinction and relight phenomena. Further developments in boundary conditions are also needed.
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Appendix A

Properties of the Favre Average (Based on Reynolds Average)

The Favre average is defined as

\[
\tilde{f} = \frac{\rho f}{\rho}
\]  

(A.1)

then,

\[
\overline{\rho f} = \rho(\tilde{f} + f') = \tilde{\rho} \tilde{f} + \rho f' = \rho \frac{\rho f}{\rho} + \rho f' = \tilde{\rho} \tilde{f} + \rho f' = \tilde{\rho} f + \rho f' 
\]

thus,

\[
\frac{\rho f'}{\overline{\rho f}} = 0
\]  

(A.2)

in the mean time,

\[
\tilde{f} = \frac{\overline{\rho f}}{\overline{\rho}} = \frac{(\tilde{\rho} + \rho') (\tilde{f} + f')}{\overline{\rho}} = \frac{\tilde{\rho} f + \tilde{\rho} f' + \rho f + \rho f'}{\overline{\rho}} = \tilde{f} + \frac{\rho f'}{\overline{\rho}}
\]  

(A.3)

on the other hand, \(\overline{\rho f} = \overline{\rho} f + \overline{\rho f'} = \tilde{\rho} f \)

then,

\[
\overline{\rho f} = \tilde{\rho} f
\]  

(A.4)

by definition, we have, \(\overline{\rho f} = \tilde{\rho} f = \tilde{\rho} f \),

\[
\tilde{f} = \tilde{f}
\]  

(A.5)

another important relation is:

\[
\overline{\rho fg} = \rho(\tilde{f} + f') (\tilde{g} + g') = \tilde{\rho} \tilde{g} + \tilde{\rho} \tilde{g}' + \rho \tilde{g} + \rho \tilde{g}' = \tilde{\rho} \tilde{g} + \tilde{\rho} \tilde{g}'
\]  

(A.6)
Appendix B

Filtered G-Equation and G-Variance Equation

B.1 Derivation of Filtered G-Equation for Compressible Flows

The instantaneous G-equation can be written as follows:

$$\frac{\partial \rho G}{\partial t} + \nabla \cdot \rho u G = \rho S_L \sigma \tag{B.1}$$

where $\sigma = |\nabla G|$. After being filtered, the above equation becomes:

$$\frac{\partial \rho \tilde{G}}{\partial t} + \nabla \cdot \rho u \tilde{G} = \rho S_L \tilde{\sigma} \tag{B.2}$$

Using Favre average, Eq. B.2 becomes:

$$\frac{\partial \rho \tilde{G}}{\partial t} + \nabla \cdot \rho \tilde{u} \tilde{G} = \nabla \cdot (\rho \tilde{u} \tilde{G} - \rho \tilde{u} \tilde{G}) + \rho S_L \tilde{\sigma} \tag{B.3}$$

There are two unclosed terms in Eq. B.3:

(1) $\nabla \cdot (\rho \tilde{u} \tilde{G} - \rho \tilde{u} \tilde{G})$

This term is the turbulent transport term. According to Peters (2002), it cannot be modeled using a classical gradient transport approximation since this would result in an elliptic equation for $\tilde{G}$ and contradict the mathematical nature of the original G equation. So this term will be modeled as: $\nabla \cdot (\rho \tilde{u} \tilde{G} - \rho \tilde{u} \tilde{G}) = \rho D_t \tilde{k} |\nabla \tilde{G}|$.

(2) $\rho S_L \tilde{\sigma}$

This term is the turbulent propagation term. We introduce a turbulent flame speed term $S_T$, which leads to $\rho S_L \tilde{\sigma} = \rho S_T |\nabla \tilde{G}|$.

Then the modeled filtered G equation becomes:
B.2 Derivation of Filtered G-Variance Equation for Compressible Flows

Define $G'' = G - \tilde{G}$. From Eq. B.2 we can get:

\[
\frac{\partial G}{\partial t} + u \cdot \nabla G = S_L \sigma
\]  \hspace{1cm} (B.5)

\[
\frac{\partial \rho G}{\partial t} + \nabla \cdot \rho u G = \rho S_L \sigma
\]  \hspace{1cm} (B.6)

\[
\frac{\partial \tilde{G}}{\partial t} + \tilde{u} \cdot \nabla \tilde{G} = \tilde{S}_L \sigma
\]  \hspace{1cm} (B.7)

Using continuity equations $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0$ and $\frac{\partial \tilde{\rho}}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{u}) = 0$, from Eq. B.6

\[
\frac{\partial \tilde{\rho} \tilde{G}}{\partial t} + \tilde{\nabla} \cdot (\tilde{\rho} \tilde{u} \tilde{G}) = \tilde{\nabla} \cdot \left( \tilde{\rho} \tilde{u} \tilde{G} - \tilde{\rho} G \right) + \tilde{\rho} S_L \tilde{\sigma}
\]  \hspace{1cm} (B.8)

\[
\frac{\partial \tilde{\rho} \tilde{G}}{\partial t} + \tilde{\nabla} \cdot (\tilde{\rho} \tilde{u} \nabla \tilde{G}) = \nabla \cdot \left( \tilde{\rho} \tilde{u} \tilde{G} - \rho u G \right) + \tilde{\rho} S_L \tilde{\sigma}
\]  \hspace{1cm} (B.9)

Eq. B.7 – Eq. B.9, we get

\[
\tilde{\rho} \frac{\partial \tilde{G}''}{\partial t} + \tilde{\rho} \tilde{u} \tilde{\nabla} G'' + \tilde{\rho} u'' \nabla G = \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{G} - \tilde{\rho} G) + \tilde{\rho} S_L \tilde{\sigma}''
\]  \hspace{1cm} (B.10)

Eq. B.10 is divided by $\tilde{\rho}$

\[
\frac{\partial \tilde{G}''}{\partial t} + \tilde{u} \nabla G'' - u'' \nabla G'' = \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{G} - \tilde{\rho} G) + S_L \sigma''
\]  \hspace{1cm} (B.11)

\[
\rho \frac{\partial \tilde{u} \nabla G'' - u'' \nabla \tilde{G}}{\partial t} = \rho \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{G} - \rho u G) + \rho S_L \sigma''
\]  \hspace{1cm} (B.12)

Multiply Eq. B.12 with $2G''$:

\[
\frac{\partial \rho G''^2}{\partial t} + \nabla \cdot (\rho u G''^2) + 2 \rho u'' G'' \nabla \tilde{G} = 2 G'' \frac{\rho}{\tilde{\rho}} \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{G} - \tilde{\rho} G) + 2 \rho S_L \sigma''
\]  \hspace{1cm} (B.13)

Filter the above equation:
Rewrite the above equation:

\[
\frac{\partial \rho \left(\bar{G}^{G^2} \right)}{\partial t} + \nabla \cdot \left( \rho \bar{u} \left(\bar{G}^{G^2} \right) \right) = -\nabla \cdot \left( \rho \bar{u} \left(\bar{G}^{G^2} \right) \right) - \frac{2 \rho u^n G^n \nabla \bar{G}}{\bar{p}} + \frac{2 \rho u^n G^n \sigma^n}{\bar{p}}
\]

(B.14)

There are five unclosed terms in the above equations. Following the same method used by Peters for RANS (2000), these terms can be modeled as follows:

1. \( (1) = \rho D_i \kappa \left\| \nabla \bar{G}^{G^2} \right\| \)
2. \( (2) = 2 \rho D_i \left\| \nabla \bar{G} \right\|^2 \)
3. \( (3) = 0. \) This term can be neglected
4. \( (4) = C_a \rho \frac{A}{q_{sgs}} \bar{G}^{G^2} \)
Appendix C

Jacobian Matrices, Eigenvalues and Eigenvectors

C.1 Jacobian Matrices, Eigenvalues and Eigenvectors

Starting from the conservative form of the governing equations (Eq. 4.17):

\[
\frac{\Delta Q}{\Delta t} + E_x |_{i-1/2,j,k}^{i+1/2,j,k} + F_y |_{i,j-1/2,k}^{i,j+1/2,k} + G_z |_{i,j,k-1/2}^{i,j,k+1/2} = H_0
\]  

(C.1)

where \( Q = (\rho, \rho u, \rho v, \rho w, \rho E, \rho G)^T \) and

\[
H_0 = H - E_x |_{i-1/2,j,k}^{i+1/2,j,k} + F_y |_{i,j-1/2,k}^{i,j+1/2,k} + G_z |_{i,j,k-1/2}^{i,j,k+1/2}.
\]

Here, the superscripts in Eq. 4.17 are dropped for convenience. Note that in the present formulation (Eq. 3.32),

\[
\rho E = \rho [\psi + \int_{x_{ref}}^x C_p(T')dT' - p + (u^2 + v^2 + w^2)/2 + k_{xpr}]
\]

\[
\approx \rho [\overline{C}_p T - p + h_f + (u^2 + v^2 + w^2)/2]
\]

where \( h_f = \psi - \overline{C}_p T_{ref} \). \( k_{xpr} \) is neglected for convenience.

The non-conservative form of the governing equations is:

\[
\frac{\Delta Q}{\Delta t} + A \cdot Q |_{i-1/2,j,k}^{i+1/2,j,k} + B \cdot Q |_{i,j-1/2,k}^{i,j+1/2,k} + C \cdot Q |_{i,j,k-1/2}^{i,j,k+1/2} = H_0
\]  

(C.2)

where \( A = \frac{\partial E_x}{\partial Q} \), \( B = \frac{\partial F_y}{\partial Q} \) and \( C = \frac{\partial G_z}{\partial Q} \).

The Jacobian \( A \) is given as:
To facilitate the analysis, we define primitive variables

\[
\mathbf{A} = \begin{bmatrix}
0 & S_{\xi x} & S_{\xi y} & S_{\xi z} & 0 & 0 \\
-\mu U + S_{\xi x}(\gamma - 1) & (S_{\xi x} + U) & (S_{\xi y} + U) & (S_{\xi z} + U) & S_{\xi x}(\gamma - 1) & 0 \\
(q^2 / 2 + h_j) & (S_{\xi y} + U) & (S_{\xi y} + U) & (S_{\xi z} + U) & S_{\xi y}(\gamma - 1) & 0 \\
(-\nu U + S_{\xi x}(\gamma - 1)) & (S_{\xi x} + U) & (S_{\xi y} + U) & (S_{\xi z} + U) & S_{\xi x}(\gamma - 1) & 0 \\
(q^2 / 2 + h_j) & (S_{\xi y} + U) & (S_{\xi y} + U) & (S_{\xi z} + U) & S_{\xi y}(\gamma - 1) & 0 \\
(U[-\gamma E + (\gamma - 1)q^2]) & (S_{\xi x} + U) & (S_{\xi y} + U) & (S_{\xi z} + U) & S_{\xi x}(\gamma - 1) & 0 \\
-(\gamma - 1)U & (S_{\xi x} + U) & (S_{\xi y} + U) & (S_{\xi z} + U) & S_{\xi x}(\gamma - 1) & 0 \\
-GU & G\tilde{S}_{\xi x} & G\tilde{S}_{\xi y} & G\tilde{S}_{\xi z} & 0 & U
\end{bmatrix}
\]

where \( U = S_{\xi x} + S_{\xi y} + S_{\xi z}, \ q^2 = u^2 + v^2 + w^2. \)

The Jacobian matrices in the \( \eta \) and \( \zeta \) directions can be obtained by replacing \( U \) with \( V = S_{\eta x} + S_{\eta y} + S_{\eta z}, \ W = S_{\eta x} + S_{\eta y} + S_{\eta z} \) and the subscript \( \xi \) with \( \eta \) and \( \zeta \) in \( \mathbf{A}. \)

To facilitate the analysis, we define primitive variables \( \tilde{\mathbf{Q}} = (\rho, u, v, w, p, G)^T \). Then, Eq. C.2 can be rewritten as:

\[
\frac{\Delta \tilde{\mathbf{Q}}}{\Delta t} + \tilde{\mathbf{A}} \cdot \tilde{\mathbf{Q}} = \tilde{\mathbf{B}} \cdot \tilde{\mathbf{Q}} + \tilde{\mathbf{C}} \cdot \tilde{\mathbf{Q}} = \tilde{\mathbf{H}}_0
\]  

where \( \tilde{\mathbf{A}} = \mathbf{P}^{-1} \mathbf{A} \mathbf{P}, \tilde{\mathbf{B}} = \mathbf{P}^{-1} \mathbf{B} \mathbf{P}, \tilde{\mathbf{C}} = \mathbf{P}^{-1} \mathbf{C} \mathbf{P} \) and \( \tilde{\mathbf{H}}_0 = \mathbf{P}^{-1} \mathbf{H}_0. \)

\[
\tilde{\mathbf{A}} = \mathbf{P}^{-1} \mathbf{A} = \begin{bmatrix}
U & S_{\xi x} \rho & S_{\xi y} \rho & S_{\xi z} \rho & 0 & 0 \\
0 & U & 0 & 0 & S_{\xi x} / \rho & 0 \\
0 & 0 & U & 0 & S_{\xi y} / \rho & 0 \\
0 & 0 & 0 & U & S_{\xi z} / \rho & 0 \\
0 & S_{\xi x} \rho & S_{\xi y} \rho & S_{\xi z} \rho & U & 0 \\
0 & 0 & 0 & 0 & U & 0
\end{bmatrix}
\]
with \( P = \partial Q / \partial \tilde{Q} \) and \( P^{-1} = \partial \tilde{Q} / \partial Q \).

\[
P = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
\rho & 0 & 0 & 0 & 0 \\
\rho & 0 & 0 & 0 & 0 \\
\rho & 0 & 0 & 0 & 0 \\
st / 2 + h / \gamma & \rho u & \rho v & \rho w & 1 / (\gamma - 1) \\
G & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

\[
P^{-1} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
-\rho & 1/\rho & 0 & 0 & 0 & 0 \\
-\rho & 1/\rho & 0 & 0 & 0 & 0 \\
-\rho & 1/\rho & 0 & 0 & 0 & 0 \\
(y - 1)(q^2 / 2 - h / \gamma) & -(y - 1)u & -(y - 1)v & -(y - 1)w & (y - 1) \\
-G & 0 & 0 & 0 & 1/\rho \\
\end{bmatrix}
\]

Similar expressions can be obtained for \( \tilde{B} \) and \( \tilde{C} \).

The eigenvalues of the flux Jacobin matrix \( \tilde{A} \) are obtained by solving the following equation:

\[
|\tilde{A} - \lambda I| = 0
\]

(C.4)

The resulting eigenvalues are:

\[
\lambda_4 = \lambda_2 = \lambda_3 = \lambda_6 = U \\
\lambda_{4,5} = U \pm C
\]

(C.5)

where \( U = \tilde{S}_{\tilde{v}} u + \tilde{S}_{\tilde{w}} v + \tilde{S}_{\tilde{w}} w \) and \( C = c |\tilde{S}_{\tilde{z}}| \).

The corresponding right and left eigenvectors matrices of \( \tilde{A} \), \( T \) and \( T^{-1} \) (\( T^{-1} \tilde{A} T = \Lambda_{\tilde{z}} \)) are:

\[
T = \begin{bmatrix}
\hat{S}_{\tilde{v}} & \hat{S}_{\tilde{w}} & \hat{S}_{\tilde{z}} & \rho / 2c & \rho / 2c & 0 \\
0 & -\hat{S}_{\tilde{w}} & \hat{S}_{\tilde{z}} & \hat{S}_{\tilde{w}} / 2 & -\hat{S}_{\tilde{z}} / 2 & 0 \\
0 & \hat{S}_{\tilde{w}} & 0 & \hat{S}_{\tilde{z}} / 2 & -\hat{S}_{\tilde{w}} / 2 & 0 \\
-\hat{S}_{\tilde{z}} & 0 & \hat{S}_{\tilde{z}} / 2 & 0 & \hat{S}_{\tilde{v}} / 2 & 0 \\
0 & 0 & \rho c / 2 & \rho c / 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
\end{bmatrix}
\]
\[ T^1 = \begin{pmatrix}
\hat{S}_{\xi} & 0 & \hat{S}_{\eta} & -\hat{S}_{\zeta} & -\hat{S}_{\xi} / c^2 & 0 \\
\hat{S}_{\eta} & -\hat{S}_{\xi} & 0 & \hat{S}_{\zeta} & -\hat{S}_{\eta} / c^2 & 0 \\
\hat{S}_{\zeta} & \hat{S}_{\xi} & -\hat{S}_{\eta} & 0 & \hat{S}_{\zeta} / c^2 & 0 \\
0 & \hat{S}_{\xi} & \hat{S}_{\eta} & \hat{S}_{\zeta} & 1 / \rho c & 0 \\
0 & -\hat{S}_{\xi} & -\hat{S}_{\eta} & -\hat{S}_{\zeta} & 1 / \rho c & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix} \]

where \( \hat{S}_{\xi} = \overline{S}_{\xi} \) \( \overline{\overline{\overline{\overline{\overline{\overline{S}}_{\xi}}}}}, \hat{S}_{\eta} = \overline{S}_{\eta} \) \( \overline{\overline{\overline{\overline{\overline{\overline{S}}_{\eta}}}}}, \hat{S}_{\zeta} = \overline{S}_{\zeta} \) \( \overline{\overline{\overline{\overline{\overline{\overline{S}}_{\zeta}}}}}. \)

Then the right and left eigenvector matrices for Jacobian matrix \( A, M_{\xi} \) and \( M_{\xi}^{-1} \), can be obtained using \( M_{\xi} = PT \) and \( M_{\xi}^{-1} = T^{-1}P^{-1} \) (note: \( M_{\xi}^{-1}AM_{\xi} = \Lambda_{\xi} \)):
There are some other choices for the right and left eigenvectors matrices of $\tilde{\mathbf{A}}$, $\mathbf{T}$ and $\mathbf{T}^{-1}$. For instance:

$$\mathbf{T}^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & -1/c^2 & 0 \\ 0 & \hat{\mathbf{S}} \hat{\mathbf{S}} / \hat{\mathbf{S}} & \hat{\mathbf{S}} / \hat{\mathbf{S}} & \hat{\mathbf{S}} / \hat{\mathbf{S}} & \hat{\mathbf{S}} / \hat{\mathbf{S}} & 0 \\ 0 & 0 & 0 & 0 & 1/ho & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \end{bmatrix}$$
The corresponding right and left eigenvector matrices of Jacobian matrix $A$, $M^\xi_s = PT$ and $M^{\xi^{-1}}_\xi = T^{-1}P^{-1}$ are:

$$M^{\xi^{-1}}_\xi = \begin{bmatrix}
1 & 0 & 0 & \frac{\rho}{2c} & \frac{\rho}{2c} \\
\rho \dot{S}_{\xi_y} / \dot{S}_{\xi_x} & \rho \dot{S}_{\xi_z} / \dot{S}_{\xi_x} & \frac{\rho(u + \dot{S}_{\xi_c} c)}{2c} & \frac{\rho(u - \dot{S}_{\xi_c} c)}{2c} \\
\rho \dot{S}_{\xi_y} / \dot{S}_{\xi_z} & -\rho & \frac{\rho(v + \dot{S}_{\xi_c} c)}{2c} & \frac{\rho(v - \dot{S}_{\xi_c} c)}{2c} \\
0 & -\rho & \frac{\rho(w + \dot{S}_{\xi_c} c)}{2c} & \frac{\rho(w - \dot{S}_{\xi_c} c)}{2c} \\
\frac{q^2}{2} + h_f & \rho u \dot{S}_{\xi_y} / \dot{S}_{\xi_x} - \rho v & \rho u \dot{S}_{\xi_z} / \dot{S}_{\xi_x} - \rho w & \rho (H + \dot{U} c) w & \rho (H - \dot{U} c) w \\
G & 0 & 0 & \frac{\rho G}{2c} & \frac{\rho G}{2c}
\end{bmatrix}$$

$$M^{\xi^{-1}}_\xi = \begin{bmatrix}
1 - \frac{(\gamma - 1)(q^2 / 2 - h_f)}{c^2} & \frac{(\gamma - 1)u}{c^2} & \frac{(\gamma - 1)v}{c^2} & \frac{(\gamma - 1)w}{c^2} & \frac{-(\gamma - 1)}{c^2} \\
-\frac{(\dot{S}_{\xi_y} \dot{U} - v)}{\rho} & \frac{\dot{S}_{\xi_y} \dot{S}_{\xi_x} / \rho}{\rho} & \frac{(\dot{S}_{\xi_y}^2 - 1)/ \rho}{\rho} & \frac{\dot{S}_{\xi_y} \dot{S}_{\xi_z} / \rho}{\rho} & 0 \\
-\frac{(\dot{S}_{\xi_z} \dot{U} - w)}{\rho} & \frac{\dot{S}_{\xi_z} \dot{S}_{\xi_x} / \rho}{\rho} & \frac{(\dot{S}_{\xi_z}^2 - 1)/ \rho}{\rho} & \frac{\dot{S}_{\xi_z} \dot{S}_{\xi_y} / \rho}{\rho} & 0 \\
\frac{(\gamma - 1)(q^2 / 2 - h_f)}{\rho c} & \frac{-(\gamma - 1)u}{\rho c} & \frac{-(\gamma - 1)v}{\rho c} & \frac{-(\gamma - 1)w}{\rho c} & \frac{-(\gamma - 1)}{\rho c} \\
\frac{\rho \dot{U} / \rho}{\rho c} & \frac{\dot{S}_{\xi_x} / \rho}{\rho c} & \frac{\dot{S}_{\xi_y} / \rho}{\rho c} & \frac{\dot{S}_{\xi_z} / \rho}{\rho c} & 0 \\
\frac{\rho \dot{S}_{\xi_x} / \rho}{\rho c} & \frac{-(\gamma - 1)u}{\rho c} & \frac{-(\gamma - 1)v}{\rho c} & \frac{-(\gamma - 1)w}{\rho c} & \frac{-(\gamma - 1)}{\rho c} \\
\frac{\rho \dot{S}_{\xi_y} / \rho}{\rho c} & \frac{(\gamma - 1)(q^2 / 2 - h_f)}{\rho c} & \frac{-(\gamma - 1)u}{\rho c} & \frac{-(\gamma - 1)v}{\rho c} & \frac{-(\gamma - 1)w}{\rho c} \\
\frac{\rho \dot{S}_{\xi_z} / \rho}{\rho c} & \frac{\rho \dot{U} / \rho}{\rho c} & \frac{\dot{S}_{\xi_x} / \rho}{\rho c} & \frac{\dot{S}_{\xi_y} / \rho}{\rho c} & \frac{\dot{S}_{\xi_z} / \rho}{\rho c} \\
-G & 0 & 0 & 0 & \frac{1}{\rho}
\end{bmatrix}$$

C.2 Characteristic Variables

After neglecting the last term, Eq.4.46 can be rewritten as follows:

$$M^{\xi^{-1}}_\xi \frac{\partial Q}{\partial t} + A^{\xi}_\xi M^{\xi^{-1}}_\xi \frac{\partial Q}{\partial \xi} = 0 \quad (C.6)$$
The characteristic vector $V$ is defined as $dV = M^{-1}_\xi dQ$. Then,

$$\frac{\partial V}{\partial t} + \Lambda_\xi \frac{\partial V}{\partial \xi} = 0$$

or

$$\frac{\partial V}{\partial t} + \Gamma = 0$$

where

$$dV = M^{-1}_\xi dQ = \begin{cases} 
\hat{S}_x (dp - \frac{dp}{c^2}) + (\hat{S}_x dv - \hat{S}_x dw) \\
\hat{S}_y (dp - \frac{dp}{c^2}) + (-\hat{S}_y du + \hat{S}_y dw) \\
\hat{S}_z (dp - \frac{dp}{c^2}) + (\hat{S}_z du - \hat{S}_z dv) \\
\frac{1}{\rho c} dp + (\hat{S}_x du + \hat{S}_y dv + \hat{S}_z dw) \\
\frac{1}{\rho c} dp - (\hat{S}_x du + \hat{S}_y dv + \hat{S}_z dw)
\end{cases}$$

and

$$\Gamma = \Lambda_\xi \frac{\partial V}{\partial \xi} = \begin{cases} 
U[\hat{S}_x (\frac{dp}{d\xi} - \frac{1}{c^2} \frac{dp}{d\xi}) + (\hat{S}_x \frac{dv}{d\xi} - \hat{S}_x \frac{dw}{d\xi})] \\
U[\hat{S}_y (\frac{dp}{d\xi} - \frac{1}{c^2} \frac{dp}{d\xi}) + (-\hat{S}_y \frac{du}{d\xi} + \hat{S}_y \frac{dw}{d\xi})] \\
U[\hat{S}_z (\frac{dp}{d\xi} - \frac{1}{c^2} \frac{dp}{d\xi}) + (\hat{S}_z \frac{du}{d\xi} - \hat{S}_z \frac{dv}{d\xi})] \\
(U + C)[\frac{1}{\rho c} \frac{dp}{d\xi} + (\hat{S}_x \frac{du}{d\xi} + \hat{S}_y \frac{dv}{d\xi} + \hat{S}_z \frac{dw}{d\xi})] \\
(U - C)[\frac{1}{\rho c} \frac{dp}{d\xi} - (\hat{S}_x \frac{du}{d\xi} + \hat{S}_y \frac{dv}{d\xi} + \hat{S}_z \frac{dw}{d\xi})] \\
U \frac{dG}{d\xi}
\end{cases}$$

The first three characteristic variables describe entropy and vorticity advections. The fourth and fifth variables are associated with acoustic pressure waves. The last variable represents the advection of level-set variable.
For the alternative eigenvector matrices,

\[
dV = \mathbf{M}_\zeta^{-1}d\mathbf{Q} = \begin{pmatrix}
(d\rho - \frac{dp}{c^2}) \\
\hat{S}_\zeta \hat{S}_\zeta \, du + (\hat{S}_\zeta^2 - 1)dv + \hat{S}_\zeta \hat{S}_\zeta \, dw \\
\hat{S}_\zeta \hat{S}_\zeta \, du + \hat{S}_\zeta \hat{S}_\zeta \, dv + (\hat{S}_\zeta^2 - 1)dw \\
\frac{1}{\rho c} dp + (\hat{S}_\zeta \, du + \hat{S}_\zeta \, dv + \hat{S}_\zeta \, dw) \\
\frac{1}{\rho c} dp - (\hat{S}_\zeta \, du + \hat{S}_\zeta \, dv + \hat{S}_\zeta \, dw) \\
dG
\end{pmatrix}
\]

and

\[
\mathbf{\Gamma} = \mathbf{A}_\zeta \frac{\partial \mathbf{V}}{\partial \zeta} = \begin{pmatrix}
U(\frac{dp}{d\zeta} - \frac{1}{c^2} \frac{dp}{d^2\zeta}) \\
U[\hat{S}_\zeta \hat{S}_\zeta \, \frac{du}{d\zeta} + (\hat{S}_\zeta^2 - 1)\frac{dv}{d\zeta} + \hat{S}_\zeta \hat{S}_\zeta \, \frac{dw}{d\zeta}] \\
U[\hat{S}_\zeta \hat{S}_\zeta \, \frac{du}{d\zeta} + \hat{S}_\zeta \hat{S}_\zeta \, \frac{dv}{d\zeta} + (\hat{S}_\zeta^2 - 1)\frac{dw}{d\zeta}] \\
(U + C)[\frac{1}{\rho c} \frac{dp}{d\zeta} + (\hat{S}_\zeta \, \frac{du}{d\zeta} + \hat{S}_\zeta \, \frac{dv}{d\zeta} + \hat{S}_\zeta \, \frac{dw}{d\zeta})] \\
(U - C)[\frac{1}{\rho c} \frac{dp}{d\zeta} - (\hat{S}_\zeta \, \frac{du}{d\zeta} + \hat{S}_\zeta \, \frac{dv}{d\zeta} + \hat{S}_\zeta \, \frac{dw}{d\zeta})] \\
U \frac{dG}{d\zeta}
\end{pmatrix}
\]

The first characteristic variables describe entropy wave advection and the second and third variables represent velocities advection.