Part I

Introduction

Chapter 1

Background, Motivation and Objectives

1.1 Background

Once used solely in aviation applications, the gas turbine has evolved into a workhorse in industry and has become the premier electric power generation system for peak, base and intermediate loads. Gas turbines are compact, lightweight, easy to operate, and come in sizes ranging from several hundred kilowatts to hundreds of megawatts. Along with these improvements, there has been a global interest in clean power generation which drives the continued improvement of power systems. Improvement efforts focus on reducing emissions, improving efficiency and lowering costs without sacrificing reliability.

Consequently, there is an increased interest in the application of control to combustion. The objective is to optimize combustor operation, monitor the process and alleviate instabilities and their severe consequences. One wishes to improve the system performance, for example by reducing the levels of pollutant emissions or by smoothing the pattern factor at the combustor outlet. In other cases, the aim is to extend the stability domain by reducing the level of oscillation induced by coupling between resonance modes and combustion. As combustion systems have to meet increasingly more demanding air pollution standards, their design and operation becomes more complex. The trend toward reduced NOx levels has led to new developments in different fields. For gas turbines, premixed combustors, which operate at lower local temperatures than conventional systems, have been designed. Monitoring and control of the operating point of the process have to be achieved with great precision to obtain the full benefits of the NOx reduction scheme. For premixed combustors operating near the lean stability limit, the flame is more susceptible to blowout or flashback, whereas lean flammability limit operation leads to oscillation. Research is being carried out to reduce these dynamical problems with passive and active control methods.

1.2 Motivation

When acoustics and combustion get strongly coupled, oscillating regimes called combustion instabilities (thermoacoustic instabilities) are observed. The mechanisms leading to instability are numerous and many of them are still unknown so that there is no reliable method to predict occurrence and the characteristics of combustion instabilities without first firing the combustor. However, some insight may be gained on the mechanisms controlling the instability by developing analytical and computational modeling tools. A great deal of research – both experimental and computational – has been directed toward understanding, predicting and controlling thermoacoustic instabilities, but there has been very little agreement on the coupling mechanism between the heat release from the flame and the acoustics of the combustion chamber. This is primarily because of the complex nature of the physical process. Numerous modeling efforts have been targeted toward providing reasonably simplified solutions to this complex problem [2, 3]. A number of combustion instability mechanisms including parametric flame instabilities, hydrodynamic instabilities, pulsating instabilities and periodic extinction have been discussed by Candel [4]. There are two lines of thought prevalent with regards to mechanisms of the unsteady heat release in gas turbine combustors.

The first supports the idea that the heat release fluctuations are caused by oscillations in reactant mixture strength or mass flux and the other supports the idea of flow instabilities like vortex rollup being responsible for the heat release fluctuations. In both lines of thought, the common factor is the velocity field. The heat release couples with the acoustics because of the fluctuation in the velocity field.

Combustors in the gas turbine industry operate in the turbulent flow regime. Combustion, even without the presence of turbulence, is an intrinsically complex process involving large ranges of chemical time scales and length scales. A range of length and time scales are involved in turbulence [5] and the accurate description of turbulence is possibly one of the most difficult open problems in fluid mechanics research. Turbulent combustion results from the interaction between chemistry and turbulence [6]. A flame interacting with turbulent flow can modify the turbulence characteristics due to strong acceleration of flow through the flame front. The acceleration is induced by the unsteady heat release from the flame and because of the change in kinematic viscosity associated with temperature changes. This process can be called *flame generated turbulence*. On the other hand, turbulence itself affects the flame structure: enhances the chemical reaction mechanism, distorts the flame shape or even results in local flame quenching/extinction [7].

Experimental and analytical studies – both laminar and turbulent – have been conducted for studying the effects of fluctuation of velocity field on the heat release. Baillot et al. [8] studied vibrating flames above a cylindrical burner to examine the effect of flow perturbations on combustion dynamics. Sinusoidal variation in flow velocity were implemented and periodic distortions of the conical flame shape was studied. Bourehla and Baillot [9] compared the kinematics of the fresh gas flow into a premixed conical flame and inside the flame to show the strong coupling between the velocity perturbation and the response of the flame front. Lieuwen [10] determined the response of planar flames to an arbitrarily complex acoustic field using linear analysis. The study demonstrates that the excitation of vorticity and fluctuations in the flame speed have significant qualitative and quantitative effects on the interactions between flames and acoustic waves. Lieuwen extended the laminar model to an analysis of acoustic wave scattering by turbulent flames [11]. Angelberger et al. [12] developed a code to compute the forcing of an experimentally investigated premixed dump combustor. They demonstrated that the main effect of acoustic waves entering the combustion chamber is to create large vortices and unsteady heat release when these vortices burn. They also showed that the fluctuation of inlet equivalence ratio, caused by the fluctuating mass flow rate, has a less destabilizing effect on the combustor as compared to the purely aerodynamical mechanism due to vortex formation and combustion.

1.3 Research Objectives

Although prior CFD studies have been directed toward simulating reacting flows in combustors, no single attempt has been made toward understanding the influence of parameters such as acoustics, fluid structures and mass flow perturbations on unsteady flame dynamics. The goal of this research is to use CFD modeling to explain the dynamics of heat release mechanism in premixed laminar and turbulent combustors. A bottom-up approach has been chosen for the study and the complex interactions between flow physics and flame dynamics have been avoided in the initial phase of the study. The objective has been to investigate the effects of simpler influencing parameters first and then to graduate to the complex mechanisms. The approach chosen is documented below.

1.3.1 Research Approach

There are two main paths available in reacting flow simulation to predict unstable combustion in a burner. Simulating flow in *resonators* or *amplificators*:

Resonators (Self-excited Modes): In a resonator, a perturbation at time $t = t_0$ propagates in all directions and is not dissipated. If boundary conditions do not damp these perturbations, a mechanism for self-sustained oscillation is created. No external forcing need be applied because the flow is dominated by its own instability mode.

Amplificators (Forced Response): In flow amplificators, any perturbation induced locally in the flow at time $t = t_0$ propagates downstream and is eventually washed away at later times. If the feedback loop leading to instability can be inhibited, the flow becomes stable. It can then be excited in a forced controlled mode to measure its transfer function.

Computation of self-excited combustion process is the more challenging of the two paths mentioned above. Based on the classification of paths available, the study has been divided into three segments:

1. The simulation of the coupling mechanism between combustor acoustics and unsteady heat release from a laminar premixed flame;

2. Isolating the flame-acoustic coupling mechanism and perturbing a laminar premixed flame with mass flow fluctuations to obtain the flame transfer function;

3. Including the effects of turbulence on flame dynamics by simulating flow in a swirl stabilized turbulent combustor. This concluding part of the study also includes investigation of mass flow perturbations on flame response.

The bottom-up approach which is being followed first eliminates the effects of turbulence on combustion dynamics and a laminar reacting flow regime is chosen to study the effects of other variables on the heat release mechanism. Turbulent combustion simulation comes in as the last step in investigating the effects of turbulence on flame dynamics.

Numerical simulation of laminar premixed flames is of interest because of the following reasons:

- detailed comparisons between experiments, theory and computations can be performed;

- validation of chemical and heat transfer models becomes easier (chemistry-turbulence interaction is eliminated);
- comparative ease in studying combustion instabilities (eliminating the effects of turbulent structures).

1.3.2 Specific Areas Studied

If the point of view of implementing numerical techniques is taken into consideration, computing laminar premixed flames is the first step toward the investigation of more complex configurations. To understand the effects of other parameters like acoustics on flame dynamics, turbulent flow simulation is initially avoided and laminar premixed combustion is attempted. The complexities involved with turbulent combustion are included in the last phase of the study. The study, therefore, begins with the investigation of laminar reacting flow in a Rijke tube type combustor which exhibits self-excited modes.

I. Self Excited Combustion Instability: The Rijke Tube Combustor Reacting Flow Simulation

A CFD based model has been used to compute reacting flow in the Rijke tube combustor geometry and capture the dynamics of the resonator. The combustor inlet and outlet have well-defined acoustic boundary conditions and therefore the CFD model should be able to capture the self-excited modes (limit cycles) exactly like the real experiment, providing the right frequency and also the mode amplitude. To our understanding, not a single CFD study has been able to capture the unsteady coupling mechanism between heat release from the flame and combustor acoustics in self-driven combustors like the Rijke tube. Previous attempts at simulating reacting flow inside such combustors have either simplified the flow field or have replaced the flame by a time-varying heat source. The result has been the decoupling of the heat release process from the acoustics of the chamber. Since flame location is important in making the combustor go unstable, the emphasis of this modeling effort has been in accurately capturing the flame anchoring process on the flame-stabilizer. The flame-stabilizer has multiple flow passages and participates in preheating the premixed air-fuel mixture, resulting in flame anchoring. It is important that the heat transfer mechanism inside the honeycomb be captured by the CFD model. Capturing the heat transfer mechanism and being able to anchor the flame to the right location in the combustor, the problem is well-posed and along with the correct boundary conditions the code will yield a solution which captures any mode as soon as it gets amplified. The approach to getting the solution involves the following implementation:

- inclusion of a simplified single-step chemical kinetics mechanism,
- second order accurate space discretization and first order accurate time discretization to solve the two-dimensional governing equations to obtain time-dependent solutions to describe the flame dynamics numerically,
- sufficiently small time-steps to capture the instability growth and subsequent limit-cycling.

Results have been compared with pressure-power spectra obtained from experiments and the CFD model is to be used for future studies in the development of control mechanisms for suppressing the instability as also toward developing reduced-order models of combustion dynamics for the combustor.

II. Effect of Velocity Perturbations on a Burner Stabilized Flame: Flat Flame Combustor Reacting Flow Simulation

Upon completion of the self-excited combustor reacting flow simulation, the next step in the study has been to exclude the coupling mechanism between the combustor acoustics and the heat release process from the flame. This helps establish the relationship between unsteady heat release and velocity perturbations by forcing a combustor with controlled excitations. A prerequisite condition for forcing is that a relatively “stable” baseline regime is attained upon which forcing is subsequently applied, one such method can involve exciting the velocity field at the inlet of the burner. One advantage of attempting such a study has been the availability of an experimental combustor geometry which was designed to prevent resonant frequencies to get excited and the combustion process to remain in a stable regime. The burner itself is seen as one such part and the CFD model is to be used for determining its transfer function. The acoustics and the characteristics of combustion oscillation modes can then be determined by, say, a one-dimensional acoustic code. Forced modes are fast to compute, as compared to the self-excited reacting flow simulation, because the computational domain is smaller and less cycles are required to obtain the forced response. Unlike the self-excited mode case in which longitudinal modes are naturally captured, in this case longitudinal acoustic modes can not be predicted because these modes are created inside the chamber itself.

Since the computational requirement for simulating forced response is less stringent, the approach is to implement detailed heat transfer mechanisms as well as better implementation of numerical schemes toward capturing the flow physics. The flow in the combustor is laminar and the effects of turbulence on the flame dynamics is still not present. The investigation is being restricted to the linear regime by fixing the velocity oscillations to a value which does not result in a non-linear response from the flame. Single-step chemistry is implemented followed by multiple-step chemistry models to investigate the effect of chemical dynamics on the frequency response function (FRF). The FRF obtained by forcing the flame is a building block of acoustic models which try to predict the behavior of the combustor by decomposing it into acoustic elements [13].

III. Unsteady Turbulent Premixed Combustion: Swirl Stabilized Combustor Reacting Flow Simulation

Laminar combustion simulation that have been carried out in the first two parts of the study yield valuable information on flame-acoustic coupling mechanism and flame response to mass flow perturbations (velocity oscillations). The effects of turbulence on combustion is to be investigated in this segment of the overall study. Laminar premixed combustion yields flame speeds of the order of 20 to $100\,cm/s$ for most hydrocarbon fuels (at atmospheric pressure) and flame thicknesses of the order of $1\,mm$. In a turbulent premixed flame, the laminar flame front interacts with turbulent eddies/vortices which may have velocities of the order of tens of m/s and sizes ranging from a few mm to few meters. This interaction may lead to a strong increase of the mass consumption rate of reactants and the overall flame thickness can also increase. Most combustion instabilities are the result of the coupling between unsteady combustion process and acoustic waves propagating in the combustion chamber. Even when flames are not submitted to strong combustion instabilities, acoustic waves interact with turbulent combustion and can modify flames significantly. The effect of acoustics on turbulent combustion can be both significant and very different from the effects of turbulence, so a proper description of turbulent combustor must incorporate effects of acoustic waves. Therefore, flame/acoustics interaction is simulated using a CFD model which is able to capture the flow physics, chemistry-turbulence interaction and heat transfer mechanisms accurately.

Along with flame response to inlet velocity perturbations, the effect of swirl is investigated. Swirl stabilized combustion is chosen because of its wide scale implementation in the gas turbine industry toward keeping combustion chambers compact by increasing flame compactness. The CFD code chosen is based on Large Eddy Simulation (LES) approach to solving turbulent reacting flows. This approach has been chosen because of the central difficulty associated with turbulent premixed combustion studies in predicting the shapes of vortices, their frequencies and their effects on the burner. Improving predictive capabilities for combustion instabilities simulation requires numerical methods which can compute large-scale vortices in reacting flow. LES is one such method and is a useful tool to address combustion instabilities problems and flame transfer computations.

The implementation involves addressing the following issues:

- LES subgrid scale models should be available for both the flow and turbulence-chemistry interactions,
- boundary conditions must be able to handle acoustic waves properly: the ability to simulate impedances at inlets and outlets has to be present,
- detailed modeling of combustion chemistry is required so as to eliminate the stiffness associated with single-/two-step mechanisms.

The above mentioned issues are accounted for in the modeling effort. The FRFs obtained from the computations are compared with experimentally obtained ones. As was the case in the laminar flame dynamics part of the study, investigation of turbulent flame dynamics is also directed toward the development of reduced order flame dynamics models. Numerical modeling carried out in this part of the study will help clarify the role and importance of turbulence on flame dynamics.

1.4 Organization of the Document

The dissertation document is divided into four parts, namely introduction, laminar flame dynamics studies, turbulent flame dynamics studies and conclusions and recommendations. Each part of the dissertation has been further divided into chapters. Chapter 1 introduces the issue of thermoacoustic instabilities in gas turbine combustors and discusses the motivation behind the research pursued. The research objectives are subsequently described in the last section. Chapter 2 introduces the methods applied in computational fluid dynamics

(CFD) studies of reacting flows, in particular the different techniques that can be applied. The finite volume method is briefly reviewed followed by modeling techniques for chemistry and heat transfer. Turbulent combustion modeling is introduced and large eddy simulation (LES) of turbulent reacting flows and turbulence-chemistry modeling methods are described. Literature survey conducted in the thermoacoustic instabilities field is included in Chapter 3. Past research leading to the current state of art in combustion instabilities studies are discussed and recent work leading to acoustic-flame interactions and effect of turbulence on flames is described. Modeling techniques applied in premixed combustion directed toward acoustic wave interactions with flames is reviewed.

In Chapter 4, laminar flame dynamics of a self-excited Rijke type tube combustor is investigated. The technical approach followed in the investigation of the non-linear phenomena is discussed. Accompanying experimental studies are also included in the chapter followed by description of the CFD model and the results from the simulation. Observations of the non-linear power spectrum of pressure is included in the last section. The flat flame present in the Rijke tube combustor is further investigated in Chapter 5. Linear stability analysis of the flat flame is performed and the frequency response function (FRF) between unsteady heat release rate from the flame and incoming velocity oscillations is computed by a new CFD model. The CFD model is described in detail and the observations from the simulation are recorded. Chapter 6 discusses the improvements to the CFD model proposed in Chapter 5 and includes the improved results from the newer model. The low frequency resonance phenomenon observed in experimental studies of the flat flame is investigated by a heat transfer model. At the end, the effect of changing the fuel from methane to propane on the FRF is briefly discussed.

Chapter 7 includes description of the turbulent swirl combustor and the cold flow simulation results for the combustor, along with unsteady RANS simulation of the swirl stabilized combustor. Chapter 8 contains LES of a swirl stabilized turbulent premixed flame. Effect of incoming velocity oscillations on the turbulent flame is described and vortex-flame interaction is investigated. Further investigation of the flame is carried out by URANS modeling.

Chapter 9 summarizes the work carried out and includes the conclusions from different parts of the work. Future possibilities for continuing the current research is also discussed. Appendix A briefly describes a CFD study of fuel-air mixing in a DOE combustor fuel nozzle carried out under a STTR project whereas Appendix B describes the second phase of the STTR project's work that involves the pre-design of a bluff body combustor using CFD analysis. Appendix C includes a MATLAB code for calculating the frequency response function (FRF) between two variables.