Part III

Turbulent Flame Dynamics Studies

Chapter 7

RANS Simulations: Turbulent Swirl Combustor

7.1 Rationale and Objectives

Lean premixed prevaporized (LPP) and lean direct injection (LDI) combustors are being developed to match international emission standards. LPP and LDI combustors have reduced NOx production but are susceptible to combustion instabilities [102]. Acoustic waves in the combustor perturb heat release by generating fluctuations in flame surface [103] and/or mixture fraction. If this unsteady heat release couples with acoustics, some eigenfrequencies of the combustor may be encouraged depending on the phase lag between acoustic waves and unsteady combustion. Understanding and preventing the resulting resonances are important issues in the development of LPP combustors.

Linear acoustics are used to analyze and model combustion-acoustic interactions. These models are used to predict self-sustained frequencies in gas turbine combustors [38]. In these models, the flame is viewed as a source of heat release rate oscillations which is dependent on local acoustics. These simple interaction models usually comprise of a frequency dependent transfer function, relating heat-release fluctuations with velocity fluctuations. The transfer functions are not only dependent on frequency, but also depend on the combustor geometry, operation mode of the combustor and on the interaction of vortices with the flame front. Derivation of the FRFs is possible using analytical calculations for simple combustor configurations (as derived for the flat flame in chapter 6), but the use of analytical models to obtain transfer functions for complex combustion systems have met with very limited success [2].

Both experimental and analytical studies of turbulent flame dynamics have been undertaken by researchers. In the case where the ambient flow field is highly turbulent, Vaezi and Aldredge [104] noted that for sufficiently high-turbulence levels, the appearance of the thermoacoustic instability did not result in additional acceleration of the flame front. This is in contrast to the case where the ambient flowfield is quiescent (or, in the case of laminar flow), where the thermoacoustic instability results in substantial flame front acceleration (as in the Rijke tube combustor). In the case of the laminar flat flame study (see chapters 5 and 6), substantial flame front acceleration was observed because of the applied u' perturbation. Lieuwen [11, 105] performed analytical studies to investigate the characteristics of wave interactions with wrinkled, turbulent flames with randomly moving fronts. The theory proposed predicted that a coherent, harmonically oscillating wave incident on a flame generates scattered coherent and incoherent disturbances.

Unsteady reactor models (like the WSR – well stirred reactor – models) have been used to study kinematically driven instabilities in multistep chemical mechanisms as well as extinction and ignition phenomenon [106]. Janus and Richards [107] used models based on interactions between acoustic oscillations and a distributed reaction zone to describe the dynamics of a lean premixed combustor. Using the unsteady WSR equations, they determined the response of unsteady heat release to perturbations in pressure, reactants mass flow rate, and equivalence ratio. These analyses assumed that the reactor residence time was fixed – oscillations in reacting mixture composition or temperature did not affect the residence time. The effects of neglecting these variations could be substantial in the case of complex combustion systems, especially for flames in more realistic geometries, such as ducted flames stabilized at rapid expansions or on bluff-bodies. At VACCG, two CFD studies have been performed in the past to investigate the effect of varying reacting mixture composition on thermoacoustic instabilities (see Appendix A) and to design a high pressure combustor consisting of a flame stabilized on a bluff-body (see Appendix B).

The principle distinction between the current approach of creating a FRF by applying CFD and WSR based modeling is the introduction of a length scale associated with the physical size of the combustion region. Becker and Gunther [108] were one of the first researchers to propose a model to create a flame transfer function for a premixed jet flame. Marble and Candel [109] subsequently performed analytical studies involving transfer function based analysis of turbulent flames in large combustors. Their investigation considered the interaction of a flame stabilized in a combustor where the flame was inclined to the flow so that the resultant flowfield was two dimensional. The analysis was also motivated by the fact that self-excited combustor oscillations in many systems occur at low frequencies where chemical kinetic processes do not influence the dynamics of the interaction. The essential approach used in their study involved matching acoustic oscillations, assumed to be one dimensional, using jump conditions. The study showed the importance of considering a finite sized flame region in accounting for the interactions between acoustic disturbances and the flame front.

Analyses by most investigators [2, 8] show that the flame exhibits a strong response to acoustic velocity perturbations. These studies all assumed that the local velocity perturbations were one dimensional. A planar incident wave impinging on a multidimensional flame front not only generates planar reflected and transmitted waves, but also multidimensional disturbances that are generally evanescent for the frequencies of interest. Lee and Lieuwen [110] argued that calculations of the flame's interactions with the acoustic field must account for multidimensional characteristics. The computational study of the acoustic near field of the flame showed that the acoustic velocity could exhibit substantial multidimensional characteristics.

Numerous experimental investigations [38, 13, 111] have demonstrated the substantial interactions between premixed flames with intrinsically unstable or acoustically forced coherent vortical structures. Two primary mechanisms of heat release modulation by these structures have been identified: flame area modulation or large-scale entrainment of reacting mixture that burns in a rapid burst downstream of the flame location. The former interaction is similar to the heat release perturbations induced by acoustic velocity perturbations. The two interaction methods have been described in detail by Schadow and Gutmark [112] and Coats [113].

The present investigation focuses on relating the incoming mass-flow oscillations (in the form of a planar acoustic wave – fluctuations are only imposed in the u velocity) to the unsteady heat release rate of a swirl stabilized turbulent premixed flame. The study does not make any assumptions of planar acoustic behavior inside the flame front or at any downstream location. Instead, time integration of the reacting Navier-Stokes equations over the combustor geometry is pursued to capture the reacting flowfield and the acoustics of the combustion chamber. To compare results from the CFD study with experiments, data from experimental studies performed on a swirl stabilized turbulent combustor at VACCG have been used. The experimental combustor is shown in Figure 7.1. In order to simulate reacting flows in the combustor, accurate cold-flow solutions should be generated a priori. The cold flow solution is used as an initial condition for the reacting flow solution process. Therefore, efforts in modeling of the swirling cold flows were first initiated. The reacting flow CFD study augments the experimental studies performed on the swirl combustor and provides further insights in understanding of the flame dynamics and for clarifying essential physics for reduced order modeling.

7.2 Cold Flow Simulations

Initial simulations indicated that usage of turbulence models such as the k-ε model does not yield accurate solutions because of their inability to capture anisotropic turbulence present in

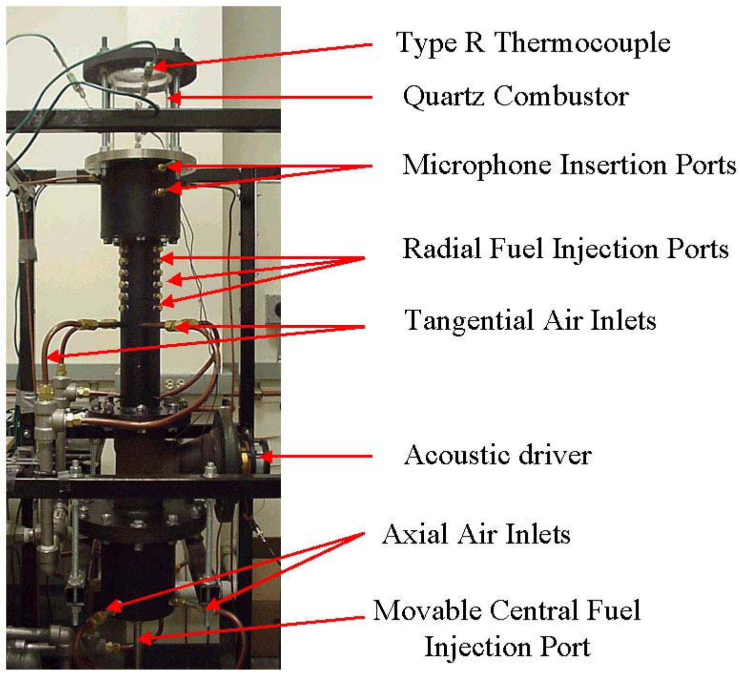

Figure 7.1: The turbulent swirl combustor

swirling flows. Using the RNG k-ε model and the Reynolds Stress Model (RSM), cold flows were simulated for the combustor illustrated in Figure 7.1. These two models are capable of capturing anisotropic turbulence to a better degree as compared to the k-ε model [114]. It was observed in literature [115] that the RNG model is more responsive to the effects of rapid strain and streamline curvature than the standard k-ε model, resulting in better performance of the RNG model for flows with weak to moderate swirl ($S < 0.5$). The effects of strong turbulence anisotropy can be modeled rigorously only by the second-moment closure adopted in the RSM [116, 117].

The first effort at modeling cold flows were initiated using the Fluent 5.1 segregated solver (FLUENT/UNS [63]) by creating a 3-D unstructured tetrahedral grid inside the combustor geometry. Various geometries were developed over a period of time before an agreement was reached on the combustor height to be used for the final simulation. The height of the combustor (the quartz chimney seen in 7.1) was selected so as to avoid combustor resonance frequencies in the present study's frequency range of interest. Figure 7.2 shows the internal features of the experimental setup that was used for the 3-D study. The long section provided downstream of the settling chamber (up till the swirler section) is to insure that the flow becomes purely axial. The port for the loudspeaker present in the experimental setup was not included in the computational geometry so as to reduce the complexities involved in numerical modeling. However, it was necessary to perform a full 3-D investigation of the flowfield inside the geometry since the swirler section prevents the application of a 2-D axisymmetric solution. To decrease computation time, the upstream section of the swirler was replaced by a computational inlet $2\,cm$ upstream of swirler where an inlet velocity boundary condition was applied.

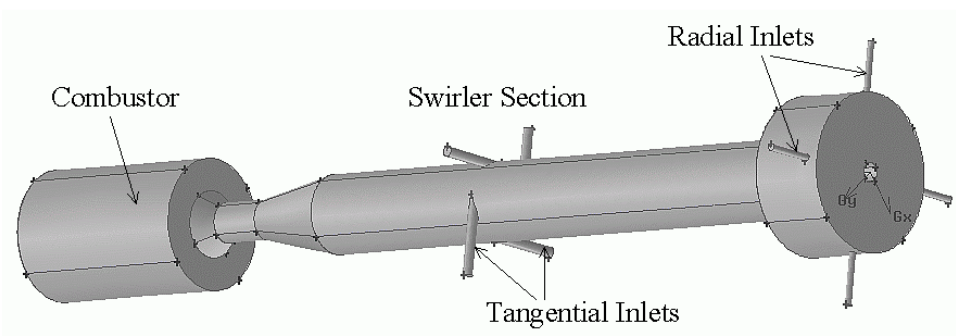

Figure 7.2: Swirl combustor internal geometry created for numerical modeling (not to scale)

A quarter of the complete geometry was used for the simulation with periodic boundary conditions. A tetrahedral mesh was generated using GAMBIT. Mass flow inlet boundary conditions were used for both the axial (radial ports) and tangential inlets. A pressure exit boundary condition was used at the combustor outlet. To avoid divergence of the initial solution because of high strain rates, laminar flow was first simulated. Using the laminar solution as an initial condition, the k-ε model was applied to obtain the turbulent flowfield solution. This approach insured faster convergence times and overall computation time was reduced. Initially, pure axial flow solution was simulated. Subsequently, tangential velocities were gradually increased to achieve the desired swirling flow solution.

7.3 Reacting Flow Simulation

Figure 7.3 shows the velocity magnitude contours inside the combustor. At the inlet of the combustor geometry, the velocities are the highest because of air entering the duct from the tangential ports at high velocity. Variation of turbulence intensity inside the combustor can be seen in Figure 7.4. The highest values of turbulence intensities can be seen downstream of the tangential inlets (because of highly swirling air) and inside the quarl section.

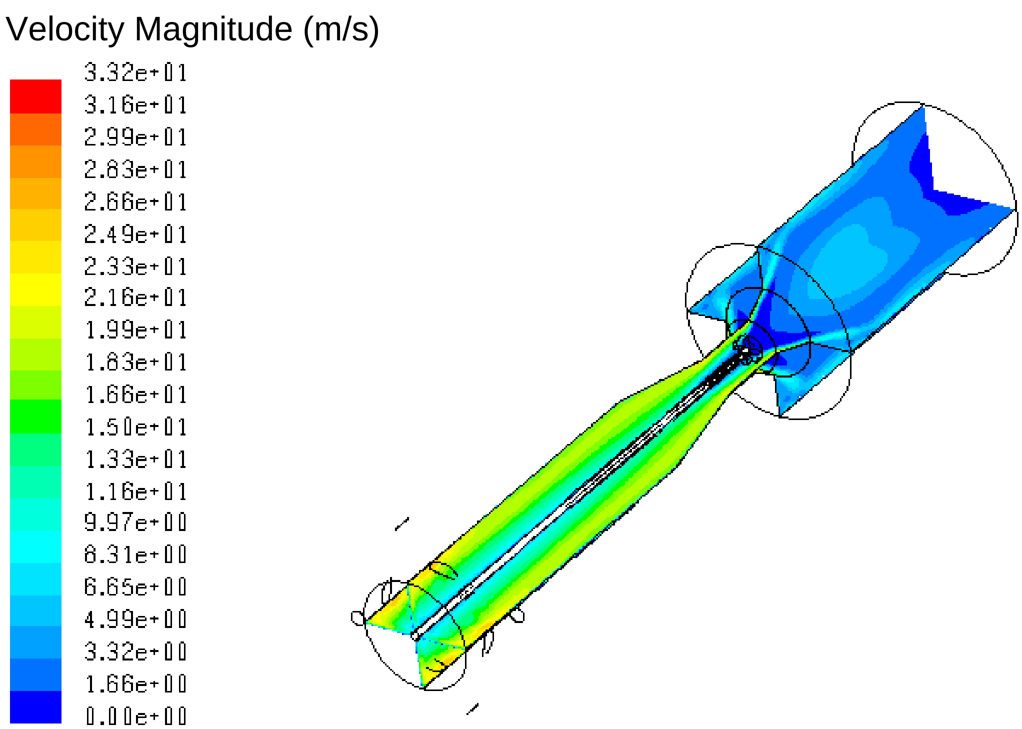

Figure 7.3: Velocity (m/s) contours inside the combustor (3D steady cold flow simulation $S_g = 1.19$, $Q = 20\,SCFM$)

At a location $2.54\,cm$ upstream of the combustor inlet, mean velocity profiles and turbu-

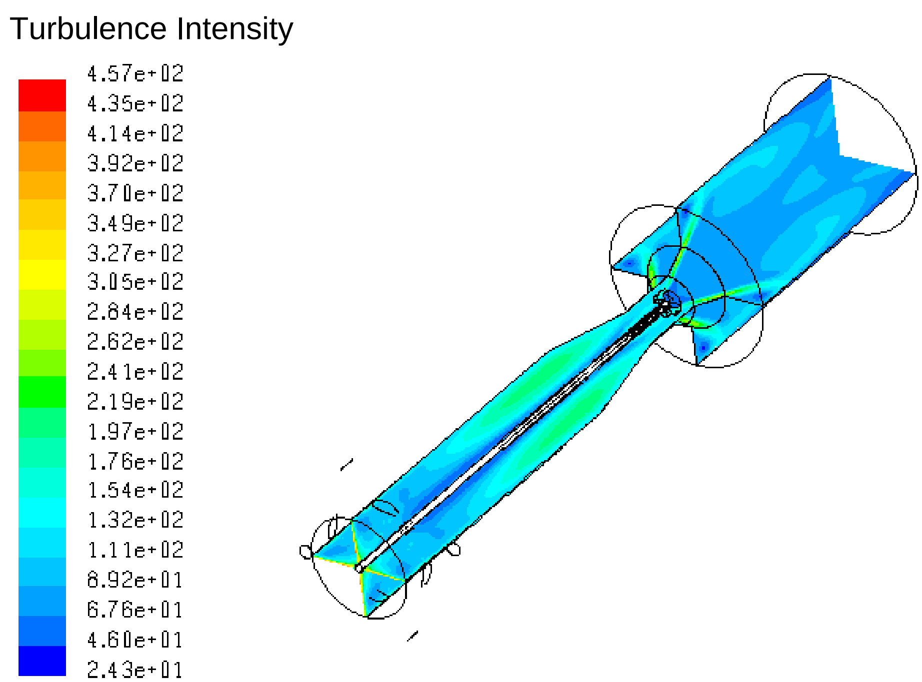

Figure 7.4: Turbulence intensity contours inside the combustor (3D steady cold flow simulation $S_g = 1.19$, $Q = 20\,SCFM$)

lence data (turbulent kinetic energy and dissipation) were measured. These profiles were subsequently used as boundary conditions for the reacting flow simulation. A steady-state reacting-flow simulation has been carried out to investigate the flame characteristics – the combustion regime, flame stabilization and flow profile inside the combustor.

Reacting flow simulation has been carried out for a 2-D axisymmetric geometry with the inlet boundary conditions obtained from the cold flow 3-D simulation. The 2-D axisymmetric calculations are computationally inexpensive compared to full 3-D reacting flow calculations. The partially premixed combustion model in Fluent 6.1 has been applied to solve the unsteady reacting flow Navier-Stokes equations (URANS). The partially premixed model was chosen because of its capability of describing the reacting flowfield with species distribution as compared to the premixed model that does not provide any information of the species. The premixed model also does not include turbulence-chemistry interactions modeling. The RNG k-ε model was used for turbulence modeling. The partially premixed model solves a transport equation for the mean reaction progress variable, $\overline{c}$ (to determine the position of the flame front), as well as the mixture fraction equations, $\overline{f}$ and $\overline{f'^2}$. The mixture fraction measures the local fuel/oxidizer ratio. Mixture fraction decouples the computations into two parts:

- A mixing part where a convection/diffusion balance equation must be solved to obtain the mixture fraction field, f as a function of spatial coordinates and time.
- A flame structure part where the relationships between flame variables (mass fractions, temperature) and mixture fraction are used to construct all flame variables. A probability density function (PDF) can be used to calculate the values of mass fractions, density and temperature for a known value of mixture fraction.

Ahead of the flame ($c = 0$), the fuel and oxidizer are mixed but unburnt, and behind the flame ($c = 1$), the mixture is burnt. Mean scalars (such as species mass fraction, temperature, and density), denoted by $\overline{\varphi}$, are calculated from the probability density function (PDF) of f and c as:

$$\overline{\varphi} = \int_0^1 \int_0^1 \varphi(f, c) df dc \tag{7.1}$$

The chemistry calculations and PDF integrations for the burnt mixture are performed in prePDF, and look-up tables are constructed for use by FLUENT. A PDF for six species (CH_4, O_2, CO, CO_2, H_2O and N_2) was generated using the prePDF 4.0 software to account for the turbulence-chemistry interactions. Figure 7.5 shows the shape of the beta PDF generated along with the chemical equilibrium distribution of instantaneous density, temperature and mole fractions of species.

Steady state results were initially obtained for the $\phi = 0.75$, $S = 1.19$ and $Q = 20\,SCFM$. Figure 7.6 shows the flame shape in terms of the reaction progress variable (c). The color blue

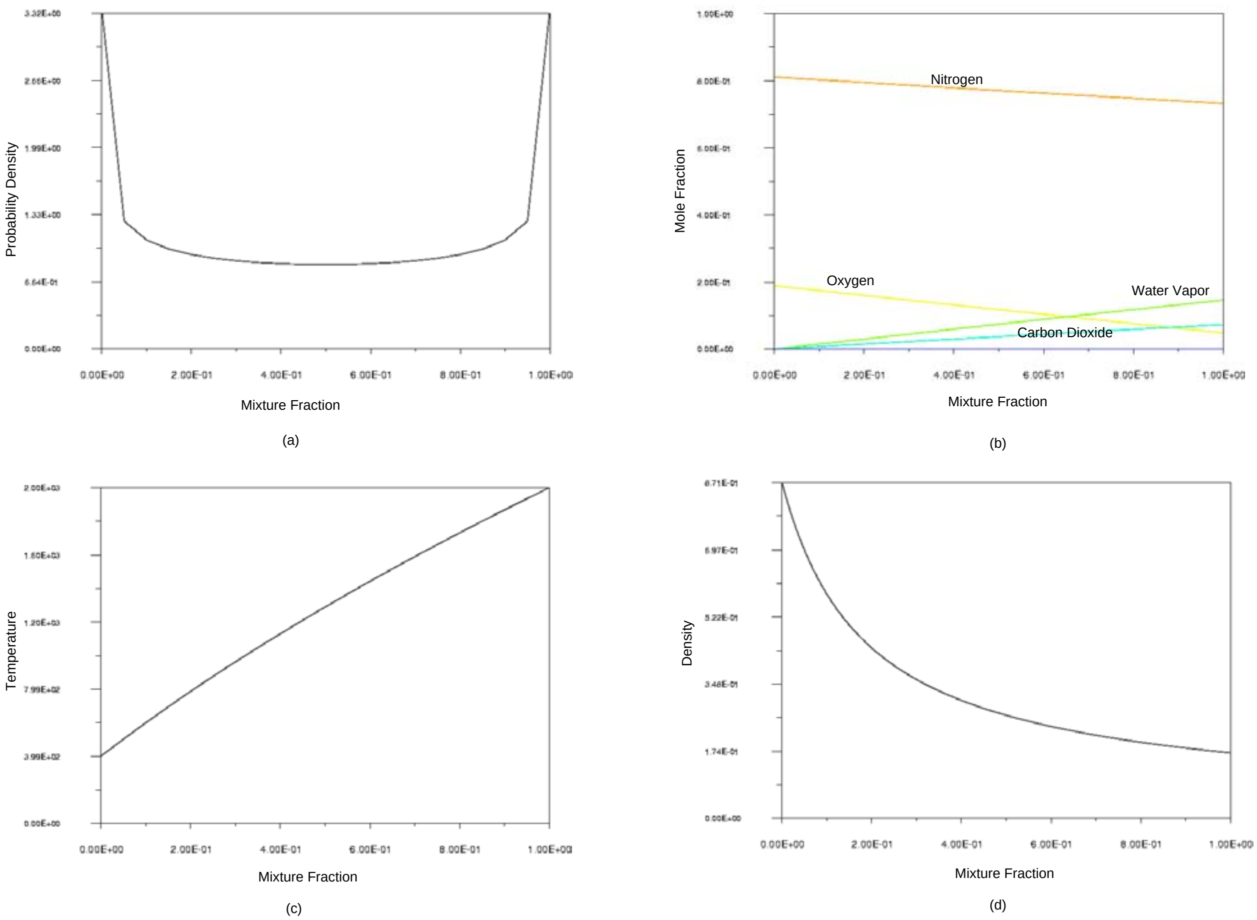

Figure 7.5: Two point Probability Density Function (PDF) generated by prePDF: (a) Beta PDF, (b) Chemical equilibrium instantaneous species composition, Chemical equilibrium instantaneous temperature (K), (d) Chemical equilibrium instantaneous density (kg/m^3)

corresponds to $c = 0$ meaning unburnt mixture whereas the color red corresponds to $c = 1$ and completely burnt products. The flame is attached on the quarl wall and extends into the combustor. Figure 7.7 shows the Damkohler number distribution inside the combustor. It can be observed from the figure that for the swirl stabilized flame, the Damkohler number is greater than one but always less than $O(10)$. The combustion category falls between the well stirred reactor (WSR) and the distributed reaction zones (see section 2.3.3 for a

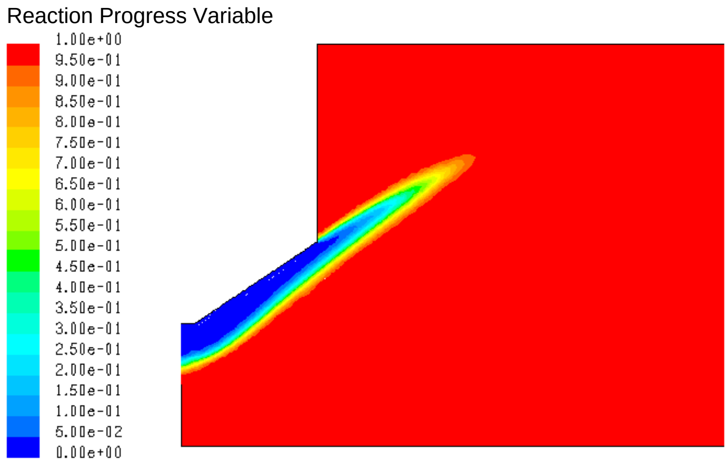

Figure 7.6: Contours of reaction progress variable from RANS simulation of the turbulent combustor ($\phi = 0.75$, $S_g = 1.19$ and $Q = 20\, SCFM$) showing unburnt ($c = 0$) and burnt ($c = 1$) regions in the combustor. The flame shape corresponds to the region between $c = 0$ and $c = 1$

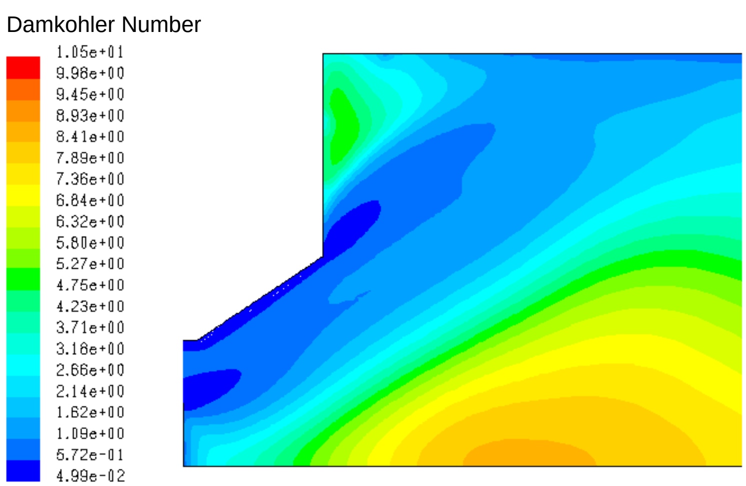

Figure 7.7: Damkohler number distribution inside the combustor – URANS simulation of the turbulent combustor ($\phi = 0.75$, $S = 1.19$ and $Q = 20\, SCFM$)

detailed explanation). The Damkohler number distribution is an indicator of the need to model turbulence-chemistry interactions using rigorous methods. In order to capture the strong effect of turbulence on the inner reaction zone of the flame two point PDF modeling is not sufficient and detailed modeling of the phenomena has to be incorporated.

In order to get a preliminary understanding of the combustion phenomena in the swirl stabilized combustor, 2D axisymmetric RANS calculations have been performed. As an initial study of flow forcing of the turbulent combustor, unsteady RANS (URANS) calculations have also been performed and discrete frequencies of excitation were applied to the swirl stabilized flame. Integrated rate of product formation was chosen as the heat release rate indicator. FRF between unsteady velocity oscillations and the unsteady heat release rate have been obtained. Figure 7.8 shows the magnitude and phase of the FRF. Around $10\,dB$ decrease in magnitude is observed between $30\,Hz$ and $500\,Hz$ with a corresponding phase drop of approximately 180°. The magnitude and phase do not show any correspondence and the $10\,dB$ drop in magnitude indicates the absence of any dynamics in the system. Since URANS involves turbulence modeling using averaged quantities (turbulent kinetic energy, k and dissipation, ε), the large scale structures in the combustor are not captured explicitly. These structures are primarily responsible for the flame dynamics. Also, the two point PDF model is not sufficient to capture the effect of turbulence on the flame. Since the Damkohler number in the flame is mostly close to one, a time accurate description of the combustion dynamics is needed to create accurate FRFs.

7.4 Summary

Unsteady RANS modeling of the turbulent flame in the swirl stabilized combustor geometry was pursued. Full 3-D cold flow simulations of a test rig provided inlet boundary conditions for the 2-D axisymmetric reacting flow simulations. A mixture fraction-PDF model was applied to capture the turbulence-chemistry interactions and the RNG k-ε turbulence model

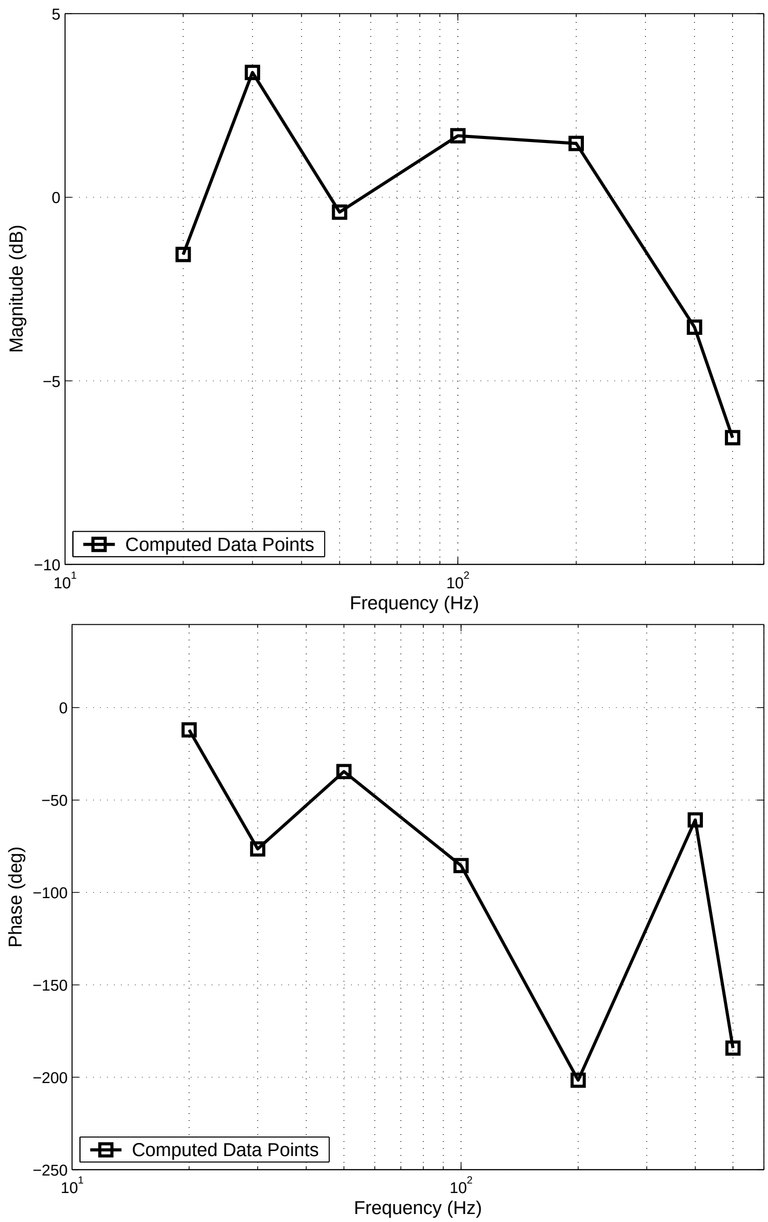

Figure 7.8: FRF magnitude and phase from URANS simulation of the turbulent combustor ($\phi = 0.75$, $S = 1.19$ and $Q = 20\, SCFM$)

was used. The reacting flow simulation showed that the flame is composed of zones of well stirred reactors (WSR) and distributed reaction zones. Therefore, rigorous modeling of the effect of turbulent mixing on chemistry needs to be implemented. A FRF between unsteady heat release rate and velocity oscillations showed zeroth order dynamics, which is unphysical. Further study of the flame dynamics process was therefore pursued using Large Eddy Simulation (LES) methodology.