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Investigation of the Mechanisms Affecting the Dynamics of Technically Premixed Flames Using LES and System Identification

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Lean premixed combustion systems are inherently more susceptible to occurrence of combustion instabilities because of the different mechanisms affecting the dynamic response of a flame. In this study, a Multiple-Input Single-Output (MISO) system identification technique will be evaluated in LES context for technically premixed-flame. The advantage of the MISO technique is that the response of flame to more than one fluctuations can be determined from single CFD simulations, leading to considerable reduction of computational cost. Furthermore, the effects of varying the fuel injection and the swirler locations on the dynamics of technically premixed flames will also be investigated. Then, the results obtained from the numerical simulations will be validated against the experimental data.

I. Introduction

In last few decades the industrial revolution and a rapid growth in world population have led to a very high demand of energy supply. A major portion of the world energy demand is fulfilled from the thermal power plants. The inherited draw back lies with these thermal power plants is the release of huge amount of different types of emissions e.g. CO2, NOX. These emissions cause the global warming and it leads to unpredictable climate changes. In order to reduce these emissions, international energy agency and governments have put strict regulations on emissions. Therefore, lean premixed combustion technology has been introduced to meet these regulations. The lean premixed combustion systems are inherently more susceptible to thermo-acoustic instabilities. Combustion instabilities can lead to an increase in emissions of noise and pollutants on one hand and lead to high level of pressure oscillations on the other hand that can cause the structural damages.

Combustion instability arises from interaction of system acoustic and unsteady heat release and can amplify due to feedback through one or more fluctuations of velocity, equivalence ratio, vorticity or entropy. These instabilities can be predicted and eliminated by performing stability analysis, but it requires understanding of the physical mechanisms affecting the dynamic response of the flames. The dynamic response of the flame to upstream perturbations can be represented by flame transfer function (FTF).

A number of mechanisms affecting the flame response have been investigated in different studies. Significant of them are velocity fluctuations,[1-5] equivalence ratio fluctuations,[6-13] large scale coherent structures,[14] entropy fluctuations,[11] and swirl number oscillations.[15-18]

The objective of this study is to investigate the combined effects of velocity and equivalence ratio fluctuations, and the effects of varying the swirler and fuel injection locations on the dynamics of technically premixed flames using Large Eddy Simulations. Furthermore, a Multiple-Input, Single-Output (MISO) system identification approach will be evaluated in LES context and quality evaluation of system identification models will be presented. The advantage of MISO approach is that the response of the flame to more than one fluctuations can be calculated simultaneously, from a single CFD simulation. This technique has already been used in RANS context for turbulent premixed flames,[19,20] and for laminar premixed case in combination with direct numerical simulations (DNS).[21] LES approach has been employed in present study because it gives better

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[§] Combustion Research Engineer, GE Global Research Center, Niskayuna, NY 12309, United States flame shape and flow physics for turbulent flames[22] and also it is computationally less expensive than DNS approach.

The outline of this paper is in first section a concept of LES-SI method has been presented. Then the details of combustion model, boundary conditions, and computation setup are described. In last section the results achieved so far and further work plan are summarized.

II. Background

II.1 Flame Transfer Function

The dynamic response of a flame to the upstream fluctuations can be represented in the frequency domain by the flame transfer function FTF. The general expression of FTF for velocity and equivalence ratio fluctuations can be represented by the relations presented in equation (1):

$$\mathrm{FTF_u}(\omega) = \frac{\acute{\dot{\mathrm{Q}}}/\bar{\dot{\mathrm{Q}}}}{\acute{\mathrm{u}}/\bar{\mathrm{u}}} \quad , \qquad \mathrm{FTF_u}(\omega) = \frac{\acute{\dot{\mathrm{Q}}}/\bar{\dot{\mathrm{Q}}}}{\acute{\varphi}/\bar{\varphi}} \tag{1}$$

II.2 LES-System Identification

In this study, the LES-SI method will be used to compute the flame transfer functions of a technically premixed flame. This method is extension of CFD-SI method[23] that was used to obtain FTF for turbulent fully premixed flames in RANS context. In this approach, the flame response over a range of frequencies can be identified in a single CFD run using broad brand excitation and system identification methods based on correlation analysis between the signal (velocity or equivalence ratio fluctuations upstream of burner) and the response (heat release rate within combustor). Most recently LES-SI approach has been successfully used for turbulent fully premixed flame[22,31] using Single-Input Single-Output system Identification technique. In case of a technically premixed system, when it is required to determine the response of the flame to more than one fluctuations e.g. velocity and equivalence ratio then we can employ a Multiple-Input Single-Output (MISO) approach. The advantage of this method is that only a single CFD simulation is required to calculate both the transfer functions i.e. $Fu\ (\omega)$ and $F\phi\ (\omega)$, (see Eq. 5 below).

A schematic description of CFD/SI for a Multiple-Input Single-Output model structure of a technically premixed flame is provided in figure 1.

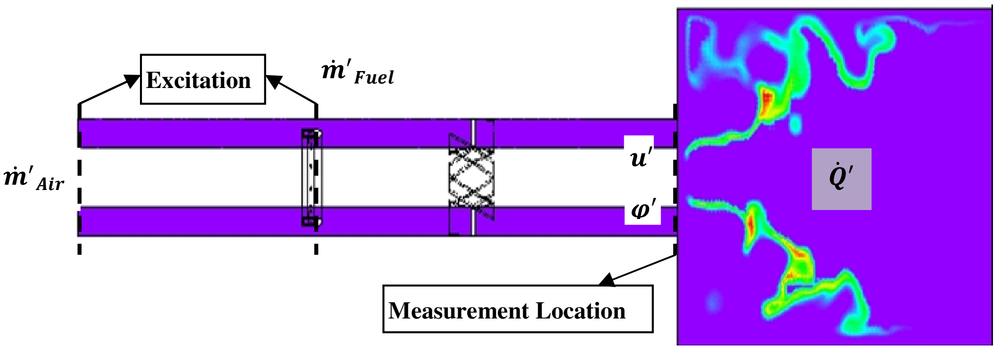


Figure 1. Multiple-Input Single-Output Model for Technically Premixed Flame

LES/SI method consists of the following steps:

- First, a simulation of the system is carried out to obtain a statistically stabilized solution.
- Then the fuel mass flow and the air mass flow are excited at the inlet boundary conditions, using broad band signals respectively. These perturbations will propagate to the flame front and create a response in the heat release of the flame.
- The area averaged velocity fluctuations and equivalence fluctuations are extracted at "measurement" planes. The heat release is obtained by a volume integration of the volumetric heat release rates in the combustor.
- These time series of signals (u',ϕ') and response (Q') are imported in a postprocessor. Then, the auto-correlation Γ and cross-correlation c of the signals are calculated. Finally, the Wiener-Hopf inversion[24] as shown in equation (2), is applied to obtain the unit impulse response h of the signals:

$$h = \Gamma^{-1} \cdot c \,. \tag{2}$$

For a technically premixed system with two input signals u', ϕ' and one response Q', the corresponding 2–1 MISO model structure in terms of UIRs of inputs signals is described as:

$$\frac{\dot{Q}'(t)}{\bar{\dot{Q}}} = \sum_{k=0}^{M} h_k \frac{u'}{\bar{u}} + \sum_{k=0}^{M} h_k \frac{\phi'}{\bar{\phi}} \quad . \tag{3}$$

Then flame transfer functions in frequency domain can be obtained by the z-transform of the unit impulse response,

$$F(\omega) = \sum_{k=0}^{M} h_k \, e^{-i\omega k \Delta t} \quad . \tag{4}$$

Then equation (3) can be written in terms of the frequency responses of the velocity and equivalence ratio fluctuations i.e. $F_u(\omega)$ and $F_\phi(\omega)$ at measurement plane as follows:

$$\frac{\dot{Q}'(\omega)}{\bar{\dot{Q}}} = F_u(\omega) \frac{u'}{\bar{u}} + F_\phi(\omega) \frac{\phi'}{\bar{\phi}} \quad . \tag{5}$$

II.3 LES Combustion Modelling

The thickness of premixed flame is about 0.1 to 1 mm and is generally much smaller than the LES mesh size, leading to a challenge for LES computation in order to resolve flame front. In this study, the Dynamic Thickened Flame Model (DTFM)[25] has been used to model turbulent flame. This model is extension of thickened flame model (TFM).[26] A deficiency lies in Thickened Flame Model is that it applies thickening in the complete domain leading to over-predicted diffusion in reactive zone by a factor F. Therefore, the Dynamically Thickened flame model[25] was introduced to overcome the deficiency of TFM. In this model a “sensor” S given by Eq. (6), is used to indicate if thickening should be applied (S=1) or not (S=0) based on the reactive zone.

$$S = tanh\left(\beta_F \frac{\Omega}{\Omega_{max}}\right) \tag{6}$$

$$\Omega = Y_F^{\nu_F} Y_O^{\nu_O} e^{-\psi \frac{T_a}{T}} \tag{7}$$

where, ψ and β_F are model constants equal to 0.5 and 500, respectively. Ψ is lower than 1 to activate sensor before reaction. Ω is a modified reaction used to activate sensor S. Ω_{max} is the maximum of Ω and it can be obtained using 1d laminar flame calculations. Finally, the sensor controls the value of thickening F given by equation (8)

$$F = 1 + (F_{max} - 1)S. \tag{8}$$

In DTFM, F is not constant, but approaches a maximum value (Fmax) inside the reaction zone and unity in non-reactive zone.[25]

II.4 Flow Solver and Computational Set-up

For the present numerical simulations, the geometry is taken from the experimental study of Ref.18. The geometry and computational setup are shown in figure 2. In order to carry out simulations, only the mixing and combustor sections are considered. The grid is three dimensional and consists of 15 millions tetrahedral elements. As the size of fuel injection holes is just 0.5 mm , so, the size of cells is 0.15 mm in this region. Furthermore, a very fine mesh is required in the region of flame and the size of the cells used in flame region is about 0.8 mm, so, a thickening factor of 7 is used on the basis of this cell size. As the thickening factor used in dynamic thickened flame model depends on the size of cells in the flame region, so, it is tried to keep the size of cells as small as possible because if thickening factor is higher, then the flame wrinkling becomes less sensitive to the turbulence, that's why a reasonable value of thickening factor should be used.

The simulations are performed using AVBP solver, developed by CERFACS. This is a compressible solver which offers a LES turbulence modelling approach to resolve large vortical structures and small scale structures are modelled using sub-grid scale (SGG) model. In these simulations the WALE (Wall Attached Layer Eddy) SGS model has been used. Furthermore, the Lax-Wendroff numerical discretization scheme is employed and it is second order accurate in space and time.

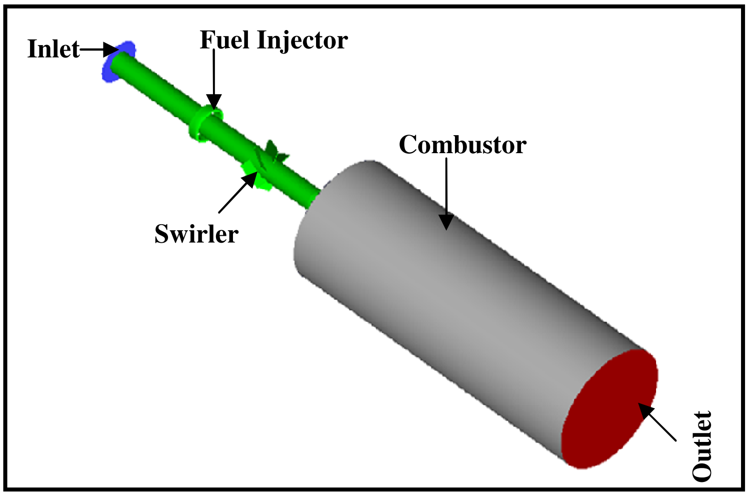


Figure 2. Set-up of The Burner for LES Simulations

II.5 Boundary Condition

The selection of appropriate boundary conditions for CFD simulations is very important to get correct results, otherwise, using inappropriate boundary conditions may introduce different types of errors in the final results. For these simulations, the inlet and outlet boundaries are imposed as non-reflective boundary conditions (NRBC).[28-30] These types of boundary conditions are necessary to use for the LES, in order to get low reflections.[32] For the combustion chamber walls, isothermal boundary condition at a constant Temperature of T=700 K is used. It has already been shown in Ref. 31 that if we use adiabatic walls it will lead to wrong stabilization of the flame. The flame shape has strong effect on flame dynamics and then definitely it will lead to a wrong prediction of flame dynamics and overall result is the incorrect prediction of stability of the given combustor.

For present case, chemistry is computed using a two-step mechanism for methane/air flame[27] with two reactions and six species as follows:

$$CH_4 + \frac{3}{2}\mathrm{O_2} \rightarrow \mathrm{CO} + \ 2\mathrm{H_2O} \tag{9}$$

$$\mathrm{CO} + \frac{1}{2}\mathrm{O_2} \leftrightarrow \ \mathrm{CO_2} \tag{10}$$

The first reaction is irreversible and rate of reaction is calculated as follows:

$$q_1 = A_1\left(\frac{\rho Y_{CH_4}}{W_{CH_4}}\right)^{n_1{}^{CH_4}}\left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{n_1{}^{O_2}} exp\left(-\frac{Ea_1}{RT}\right) \tag{11}$$

The second reaction is reversible with an equilibrium between CO and CO_2 in the burnt gases. The rate of reaction is given as follows:

$$q_2 = \left[\left(\frac{\rho Y_{CO}}{W_{CO}}\right)^{n_2{}^{CO}}\left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{n_2{}^{O_2}}\left(\frac{\rho Y_{CO_2}}{W_{CO_2}}\right)^{n_2{}^{CO_2}}\right] exp\left(-\frac{Ea_2}{RT}\right) \tag{12}$$

The reason of using this scheme is that in present case the inlet temperature is higher than the atmospheric condition i.e. T=473 K, and one step mechanism does not calculate the right value of laminar speed (S_L) and S_L is one of the important parameters to compute the response of flames because overall heat release rate and flame surface area are functions of laminar flame speed S_L.

III. Results and Discussion

In first step, steady state simulations are carried out for technically premixed combustor. In this step it is ensured that perfect mixing of air fuel and right flame shape are achieved. The results presented below are for U= 40 m/s and phi= 0.65. The results of mass fraction of methane Y_{CH4} and corresponding iso-surface are presented in figures 3(a) & 3(b). From these figures it is very clear that mixture is uniformly mixed and iso-surface is plotted for a mean value of Y_{CH4} =0.0365 for phi=0.65. These figure show that more than 95% of the inlet of combustor is receiving uniformly mixed air-fuel.

Figure-4(a) presents a comparison of experimentally and numerically computed flame structures and figure-4(b) presents a comparison of normalized spatial heat release distribution for technically premixed case. This shows that the results of LES are in very good agreement with experimental results. In order to compare the results of LES and experiment, it is important to get the right flame shape because a different flame shape can affect the flame transfer functions.

Once the right steady state flame is achieved, then the following the next steps are planned to perform:

- The simulations of the system excited with broadband signals are already in process. Two signals have been imposed, one signal to excite the flow rate of air and second one to excite the flow rate of fuel. Then the results achieved from these simulations will be used to compute the flame transfer functions i.e. $Fu(\omega)$ and $F\phi(\omega)$ using Multiple-Input Single-Output system identification technique.
- Furthermore, the harmonic excitation method will be used to analyze the effects of varying the swirler and fuel injection locations on dynamics of technically premixed flames. As it has already been shown in experimental work[18] that the acoustic and convective waves (swirl strength and equivalence ratio) interference mechanisms have considerable effects on system stability, so, the results achieved from these simulations will be validated against the experimental results of this study.

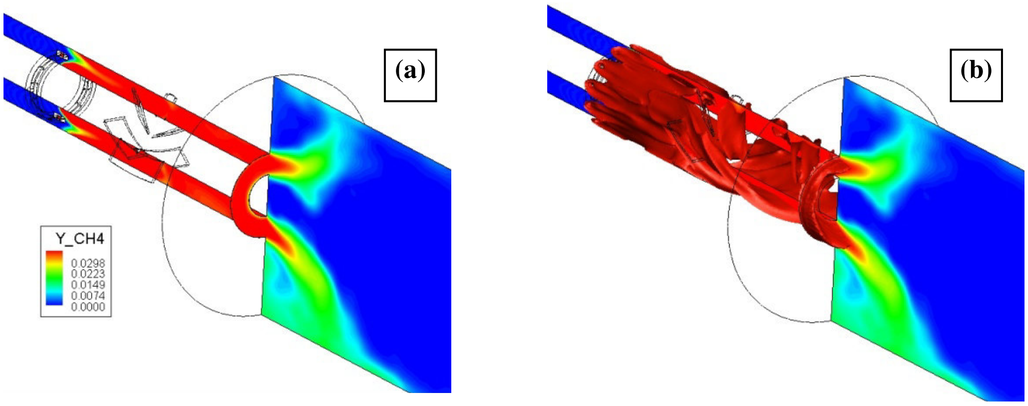
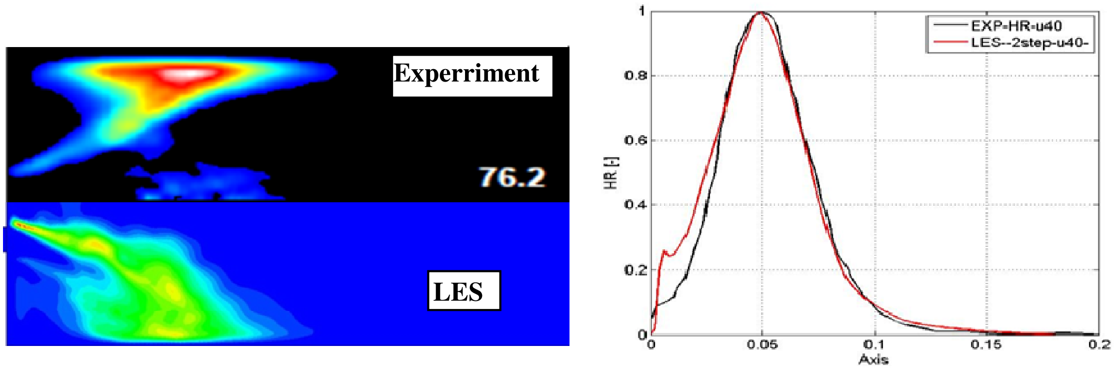


Figure 3. (a) Contours of Mass Fraction of Methane (b) Iso-Surface of Mass Fraction of Methane



(a) (b)

Figure 4. (a) Mean Heat Release from LES and OH* Chemiluminescence from Experiments (b) Comparison of Mean Axial Heat Release Distribution for LES and Experiments

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