Identification of the dynamics of technically premixed flames as multiple-input, single-output systems from LES

A. Ulhaq,* C. F. Silva, W. Polifke

Fachgebiet für Thermodynamik, Technische Universität München, 85747 Garching, Germany

If thermo-acoustic instabilities develop in a technically premixed combustion system, equivalence ratio fluctuations are likely to occur in addition to velocity fluctuations. Therefore, in this type of system, the unsteady heat release rate should be related not only to velocity perturbations upstream of the flame but also to fluctuations of the equivalence ratio. In the present work, the flame response to both velocity as well as equivalence ratio fluctuations is assessed through Large Eddy Simulation (LES). Considering the flame as a multiple-input, single-output(MISO) system, two transfer functions are deduced for a wide range of frequencies from a single LES run. Uncertainty quantification of system identification allows to compute confidence intervals for the flame transfer functions.

1. Introduction

Lean premixed combustion systems are inherently 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 acoustics with unsteady heat release and can be amplified due to feedback that involves fluctuations of velocity, equivalence ratio, vorticity or entropy. Significant are velocity fluctuations,[1, 2, 3] equivalence ratio fluctuations,[4, 5, 6] large scale coherent structures[7], entropy fluctuations [8], and swirl number oscillations[9, 10, 11]. Thermo-acoustic stability analysis requires understanding and quantitative description of the physical mechanisms affecting the dynamic response of the flame, which may be represented in terms of a flame transfer function (FTF)

In a technically premixed combustion system, in addition to velocity fluctuations, equivalence ratio fluctuations are likely to occur. The objective of this study is to investigate the combined effects of velocity and equivalence ratio fluctuations, and fuel injection locations on the dynamics of technically premixed flames using Large Eddy Simulation (LES). Furthermore, a Multiple-Input, Single-Output (MISO) system identification approach is used in LES context. 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[12, 13] and for laminar premixed case in combination with direct numerical simulations (DNS)[14]. Furthermore, the uncertainty of system identification results is presented in terms of confidence interval plots. This is of particular importance in the LES context, where the noise due to resolved turbulent fluctuations is significant.

*Corresponding author: ulhaq@td.mw.tum.de
European Combustion Meeting 2015

2. Identification of FTFs of Technically Premixed Flames

In contrast to fully premixed systems, the flame dynamics of technically premixed combustion systems is additionally influenced by equivalence ratio fluctuations. Therefore, for a technically premixed systems the correct representation of flame dynamics would require identification of both transfer functions i.e. flame transfer function $F_u(\omega)$ with respect to velocity fluctuations u' given by

$$F_u(\omega) = \frac{\dot{Q}'(\omega)}{\bar{\dot{Q}}(\omega)} / \frac{u'(\omega)}{\bar{u}(\omega)} \tag{1}$$

and a second flame transfer function $F_\Phi(\omega)$ w.r.t. equivalence ratio fluctuations Φ',

$$F_\phi(\omega) = \frac{\dot{Q}'(\omega)}{\bar{\dot{Q}}(\omega)} / \frac{\Phi'(\omega)}{\bar{\Phi}(\omega)} \tag{2}$$

where $\dot{Q}'$, u', Φ', are the fluctuations of heat release, velocity and equivalence ratio respectively and $\bar{\dot{Q}}$, $\bar{u}$, $\bar{\Phi}$ are the mean heat release, velocity and equivalence ratio [12, 13].

In a technically premixed combustion system, the equivalence ratio fluctuations are calculated by the following equation:

$$\frac{\Phi'}{\bar{\Phi}} = \frac{\dot{m}'_{fuel}}{\bar{\dot{m}}_{fuel}} - \frac{\dot{m}'_{air}}{\bar{\dot{m}}_{air}} \tag{3}$$

where $\dot{m}'_{fuel}$, $\dot{m}'_{air}$ are the fluctuations of mass flow of fuel and air and $\bar{\dot{m}}_{fuel}$, $\bar{\dot{m}}_{air}$ are the mean mass flow of fuel and air respectively. A technically premixed system can be distinguished by fuel injector types such as: stiff or non-stiff, far upstream or just close to the combustor inlet.

If a stiff fuel injection configuration is considered, then the first term on the right hand side of Eq.3 becomes zero. But it shows that even in the absence of any fluctuations of fuel mass flow rate, there still exist equivalence ratio fluctuations. In this case the equivalence ratio fluctuations are only function of upstream velocity fluctuations and these two fluctuations are fully correlated with each other. The system model for this type of configuration is summarized in Fig. 1 (top). The overall heat release fluctuations are given by the equation:

$$
\begin{aligned}
\dot{Q}'(\omega)/\bar{\dot{Q}} &= F_u(\omega)u'/\bar{u} + F_\phi(\omega)\Phi'/\bar{\Phi} \\
\Phi'/\bar{\Phi} &= F_{u,\Phi}(\omega)u'/\bar{u} \\
Q' &= (F_u(\omega) + F_\phi(\omega)F_{u,\phi}(\omega))u'/\bar{u}
\end{aligned} \tag{4}
$$

In the case of a non-stiff fuel injector, in addition to the fluctuations of air mass flow, the fluctuations of fuel mass flow are also induced by the acoustic fluctuations. Therefore, in such a configuration the equivalence ratio fluctuations are functions of both fluctuations of Eq.3 i.e. mass flow rate of air and mass flow rate of fuel. The system model for this type of configuration is sketched in Fig. 1 (bottom). Both the configurations require to model the flame as a multiple-input, single-output (MISO).

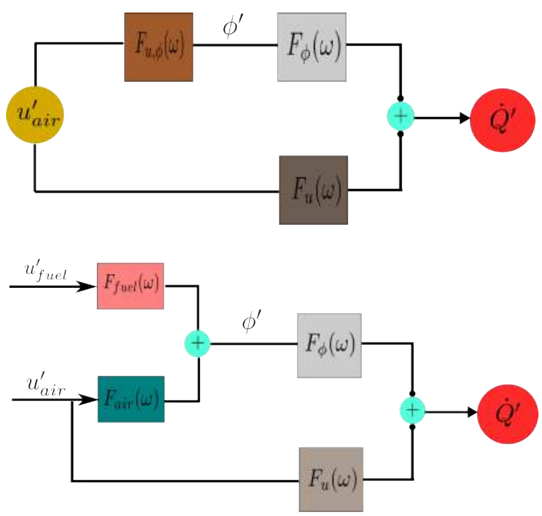

Figure 1: *Stiff fuel (top) and non-stiff (bottom) fuel injection configuration*

In Fig. 2, a flame transfer function modeling approach for technically premixed combustion system configuration is summarized depending on the upstream acoustic impedance $Z_1 = \infty$ or $Z_1 = 0$. Fuel injector is considered as "stiff" and acoustic field of the combustion system is expressed in terms of the acoustic velocity u'. In the first case for $Z_1 = \infty$, the acoustic velocity fluctuations are almost negligible at the point of measurement upstream of combustor, while it has maximum value at the point of fuel injection. In this case, a flame transfer function F_u modeled just w.r.t. upstream velocity fluctuations u' based on SISO model structure would produce no results. The reason is in this case acoustic velocity fluctuations are almost zero, while the effect of the heat release fluctuations caused by equivalence ratio fluctuations at the point of injection has been neglected.

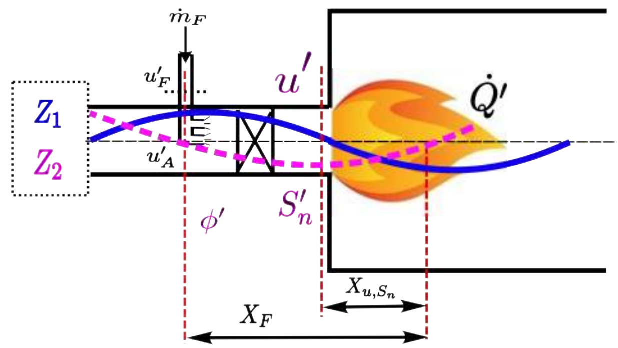

Figure 2: *Effect of acoustic impedance on modeling of FTF for technically premixed system*

In the second case when $Z_2 = 0$, the amplitude of acoustic velocity fluctuations at the point of injection is almost zero and is maximum at point of measurement upstream of the combustor. In this case, the flame dynamics based on SISO model structure can be represented because no equivalence ratio fluctuations occur. On the other hand, if fuel injector is non-stiff, then again flame dynamics based on SISO model structure would not be correct representation because of occurrence of equivalence ratio fluctuations.

Summarizing the previous ideas, we could state that in most of the cases of technically premixed flames a meaningful description of flame dynamics demands the system to be considered as MISO model structure. A MISO model structure based on the velocity and equivalence fluctuations is given by the following equation:

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

3. Flow solver and computational setup

The simulations are performed using AVBP solver, developed by CERFACS. In these simulations the WALE (Wall Attached Layer Eddy) sub-grid scale (SGS) model has been used. Furthermore, the Lax-Wendroff numerical discretization scheme is employed and it is second order accurate in space and time. The Dynamic Thickened Flame Model (DTFM)[15] has been used to model turbulent flame. Chemistry is computed using a two-step reduced scheme for laminar premixed methane/air flames called $2S\_CH4\_BFER$ [16] with six species ($CH_4, O_2, CO_2, H_2O, N_2,$ and CO).

This scheme has been validated for computing laminar flames for both lean and rich ($\Phi \leq 1.4$) regimes and also over a range of temperature and pressure values and thus suitable to perform simulations that involve equivalence ratio fluctuations.

For the present numerical simulations, the geometry is taken from the experimental study of Kim et al. [17]. In order to carry out simulations, only the mixing and combustor sections are considered. The grid is three dimensional and consists of 15 million tetrahedral elements. The diameter of fuel injection holes is 0.5 mm, with a minimum cell size of 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. A value of thickening factor 7 is used based on these cell sizes. For these simulations, the inlet and outlet boundaries are imposed as partly-reflecting boundary based on the formulation of NSCBC of Poinsot and Lele [18]. For the combustion chamber walls, no-slip adiabatic boundary condition are imposed.

4. LES/System identification (LES/SI)

In this study, LES in combination with system identification methods will be used to compute the flame transfer functions of a technically premixed flame. 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[19] 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. A schematic description of LES/SI for a MISO model structure of a technically premixed flame is provided in Fig. 3.

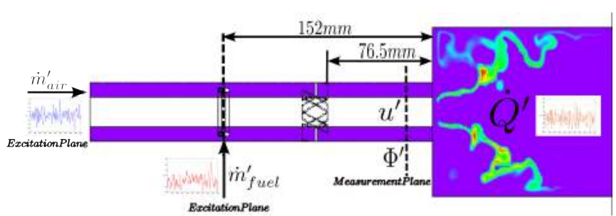

Figure 3: *LES/SI setup for technically premixed flame configuration*

In LES/SI method, firstly, a LES simulation of the system is carried out to obtain a statistically stationary solution. Then the fuel mass flow and the air mass flow are excited at the inlet boundary conditions, using broad band signals respectively. 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' and Φ') and response ($\dot{Q}'$) are imported in MATLAB. Then, the auto-correlation Γ and cross-correlation c of the signals are calculated. Finally, the Wiener-Hopf inversion, is applied to obtain the unit impulse responses (UIRs) of the signals:

$$h = \Gamma^{-1} c. \tag{6}$$

For a technically premixed system with two input signals, and one response, the corresponding 2-1 MISO model structure in terms of UIRs of inputs signals is described as [12]:

$$\frac{\dot{Q}'(t)}{\overline{\dot{Q}}} = \sum_{k=0}^{M} h_k \frac{u'}{\overline{u}} + \sum_{k=0}^{M} h_k \frac{\Phi'}{\overline{\Phi}} \tag{7}$$

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

$$F(\omega) = \sum_{k=0}^{M} h_k e^{-i\omega k \Delta t}. \tag{8}$$

5. 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 steady state flame and iso-surface of $\overline{Y}CH4 = 0.0365$ are plotted in Fig. 4 for U= 40 m/s and $\phi = 0.65$. From the figure it is clear that most of the mixture is uniformly mixed at the inlet of combustor.

Once the statistically stationary flame is achieved, then the perturbations are imposed on ingoing characteristic waves. For LES/SI, a DRBS broad band signal is used with a cut-off frequency at 1200 Hz. For both fully premixed and technically premixed case, the excitation amplitude is chosen to be an order of 8% of mean inlet velocity.

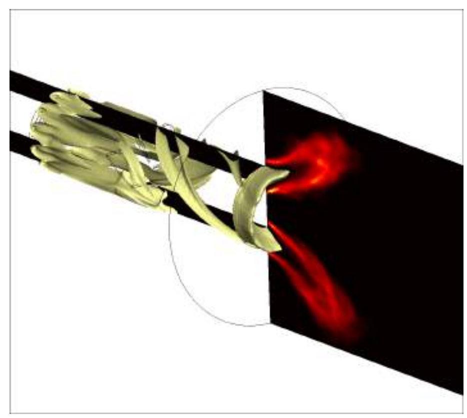

Figure 4: *Stationary flame and iso-surfaces of* $\overline{Y}_{CH4} = 0.036$

For fully premixed case, the acoustic fluctuations in the mixing section also lead to swirl fluctuations [10] and these fluctuations will affect the overall flame response by fluctuations in flame surface area. On the other hand, acoustic fluctuations in the mixing section of a technically premixed combustion system, also induce equivalence ratio fluctuations. The strength of equivalence ratio fluctuations may depend on number of factors such as: mean flow velocity, excitation frequencies and amplitudes, fuel injection location [17]. Therefore, in such a configuration the heat release response is governed by parameters such as: frequency, amplitude of velocity fluctuations(u'), amplitude of equivalence ratio fluctuations (Φ') and phase difference between u' and Φ' at the inlet of combustor [20].

In Fig. 5 a comparison of flame transfer function of fully premixed case and technically premixed case is presented. Based on the time step of Δt= 0.5e-07s, two million iterations were performed. Total simulation time is 0.1s resolving a minimum frequency of 10Hz. The acoustic velocity fluctuations (u') are recorded at a plane 10mm upstream of the combustor and heat release fluctuations $\dot{Q}$ are determined by a volume integration of the volumetric density of heat release rate over the computational domain. The gain of fully premixed case approaches to unity in low frequency limit, while the gain of technically premixed approaches to zero in low frequency limit for stiff fuel injector configuration, and in agreement with the criteria defined by Polifke and Lawn [21]. For higher frequencies the gain in both cases shows an amplification and the highest value in fully premixed case is at 200 Hz with a magnitude of 1.25, while in technically premixed case the highest value is at 180 Hz with a magnitude of 2. As elaborated in previous studies [10, 11] in a fully premixed case the magnitude and location of gain are controlled by interference mechanisms of acoustic and convective disturbances, the latter being comprised of fluctuations of swirl or equivalence ratio. The higher value of gain and variations in the gain of technically premixed as compared to fully premixed case are due to presence of equivalence ratio fluctuations and in present case these are an order of 2% of the mean Φ. In a technically premixed case the trend of overall gain depends not only on strength of velocity and equivalence ratio fluctuations but also on the phase between these two fluctuations. For the frequencies where the phase difference between these two fluctuations is zero, will lead to a constructive interference and hence the over all gain will be amplified.

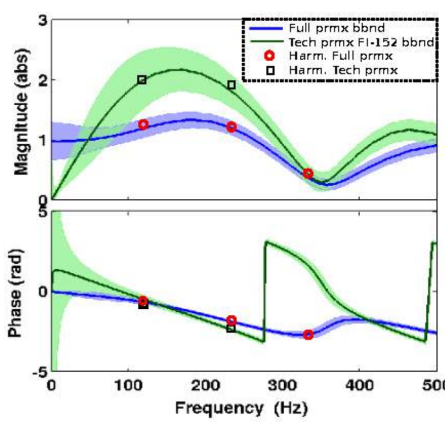

Figure 5: *Comparison of FTF for fully and technically premixed flames*

The phase plot of Fig. 5 shows that for fully premixed case it starts from zero while the phase for technically premixed case starts from a value of $-\pi/2$ radian. The phase of technically premixed case is steeper at frequencies above 100 Hz. For the present case no experimental data is available so the results are compared with the harmonic excitation method. Harmonic excitations were performed for frequencies at 110 Hz, 220 Hz and 330 Hz. Fig. 5 shows that a very good agreement between these methods.

In Fig. 6 the unit impulse response (UIRs) of both flames are displayed. The UIR_{FP} of full premixed case shows the effect of both acoustic velocity fluctuations and then with a certain time delay the effect of convective swirl fluctuations. The UIR_{TP} of technically premixed case also shows two parts. The first part is for acoustic velocity fluctuations that is similar to the fully premixed case but convective part in distinction to fully premixed case is wider and has higher strength of undershoot. This effect in convective part is the contribution of equivalence ratio fluctuations.

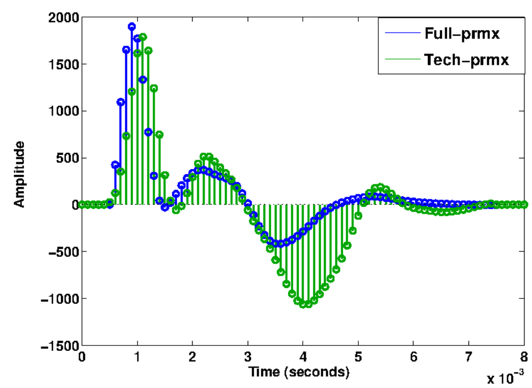

Figure 6: *Comparison of UIRs for fully and technically premixed flames*

Fig. 7 illustrates a comparison of FTFs depending on fuel injection location. In this case two fuel injection locations are considered, L_{inj} = 152 and 203mm upstream of the combustor. With L_{inj} = 203mm, the fluctuations level of equivalence ratio decreases from Φ = 2% (in case of L_{inj} = 152mm) to Φ' = 1%. The gain of FTF shows that changing the fuel injection location, the point of maximum gain has moved from 160 to 110 Hz and also magnitude of gain is smaller. The reason of this shift is that changing the fuel injection location also changes the frequency where the phase between u' and Φ' is zero (the relevant graph is not plotted here). A similar observation was also made in the experimental work of Kim et al. [17]. The phase plot shows a trend very similar to the one of fully premixed case because of low fluctuations of Φ'.

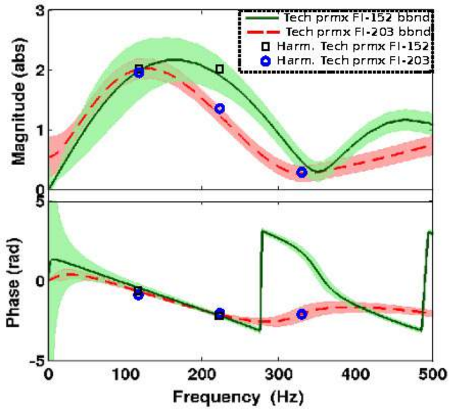

Figure 7: *Comparison of FTF for two different positions of fuel injection locations in a technically premixed system*

In the previous section, it has been shown that presence of equivalence ratio fluctuations modify the flame dynamics considerably. It can be seen from this study that for a given fixed magnitude of air mass flow fluctuations, the strength of equivalence ratio fluctuations may vary depending on the location of fuel injection location. Turbulent mixing has a significant effect on the dissipation of equivalence ratio fluctuations. If fuel injector is also non-stiff then the strength of equivalence ratio fluctuations is also modified by acoustic of the given system.

In this section, the technically premixed flame is modeled as MISO model structure, where the response of flame to both fluctuations is modeled independently. The results of $F_u(\omega)$ and $F_\Phi(\omega)$ obtained from MISO identification method are evaluated against SISO of $F_u(\omega)$ and $F_\Phi(\omega)$ respectively and also harmonic excitation methods. For MISO identification method, broad band excitation signals uncorrelated with each other are imposed on velocity of air and velocity of fuel. The excitation level for air velocity fluctuations is 10% of mean flow velocity and for fuel velocity fluctuations is 3% of mean fuel velocity. The area averaged fluctuations of velocity and equivalence ratio fluctuations are measured upstream of combustor as shown in Fig. 3.

In Fig. 8 a comparison of $F_u(\omega)$ obtained from MISO identification method is compared against SISO and harmonic methods. A good agreement is found for the gain for a frequency range between 100-300 Hz. Theoretically, the gain of FTF should approach unity in low frequency limit. However, in present case the gain of FTF obtained from MISO identification method exhibits a discrepancy. As already observed by Huber and Polifke [12] the presence of high level of noise and presence of certain level of correlation between residuals and signals can lead to such discrepancy in gain at low frequencies. Similarly, a good agreement is also found for the phase plot.

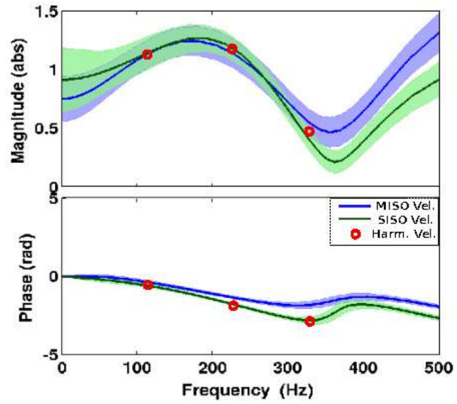

Figure 8: *Comparison of $F_u(\omega)$ for MISO and SISO and Harmonic excitation methods*

Fig. 9 provides a comparison $F_\Phi(\omega)$ from MISO identification method against SISO and harmonic methods. For gain plot a poor agreement is found with SISO, while a close agreement with harmonic excitation method is found. The phase plot shows good agreement among all three methods.

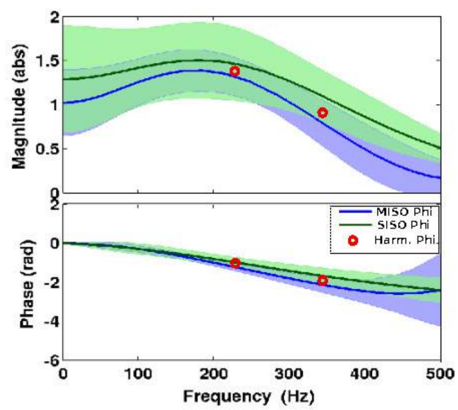

Figure 9: *Comparison of $F_\Phi(\omega)$ for MISO and SISO and Harmonic excitation methods*

Confidence intervals is one of the quality assurance parameters to analyze the reliability and statistical convergence of the identification models. The gain and phase of FTF in Fig. 8 and Fig. 9, are plotted with 70% confidence intervals. The confidence interval region of gain of $F_\Phi(\omega)$ is wider as compared to gain of $F_u(\omega)$. The reason is, the amplitude of velocity fluctuations i.e. $u' = 10\%$ is higher as compared to the amplitude of equivalence ratio fluctuations i.e. $\Phi' = 3\%$, so, giving better signal to noise ratio. The confidence interval of phase plots in both cases is narrower as compared to gain plots. Further narrower confidence interval regions can be obtained by getting a longer time series of simulations or exciting with high amplitude values. Both of them in this case are restricted as the time step of CFD simulations is really small, so, in order to get a longer time series a lot more computational resources would be required. With higher excitation amplitudes prediction quality would get better and also confidence interval region would get narrower. However, the present study is limited by the fact that an excitation level higher than 10% would lead the response in the non-linear regime. Furthermore, the prediction quality and residuals could be improved by employing identification models that also model the stochastic part of the response e.g. ARX and BJ model.

6. Conclusions

The present study explains a multiple-input, single-output (MISO) identification approach to identify the flame transfer functions i.e. $F_u(\omega)$ and $F_\Phi(\omega)$ in a technically premixed combustion systems from LES. The results of MISO model structure are validated against SISO and harmonic excitation methods and good agreement is found. Furthermore, uncertainty of system identification results is presented in terms of confidence interval plots. The confidence interval plots show poor results for the gain of flame transfer functions, while a better estimation for phase plots. The reason is presence of high noise in this configuration leads to bad signal-to-noise ratio and hence deteriorating the quality of identification. Quality of identification can be either improved by using high level of excitations and employing non-linear system identification techniques or by computing a longer time series of the simulations.

7. Acknowledgements

Financial support from higher education commission (HEC) Pakistan and Fachgebiet für Thermodynamik is greatly acknowledged. Special thanks to K. T. Kim providing details on the experimental setup. Furthermore, we are also thankful to LRZ Munich for providing computational resources for project-id: pr58gi and to CERFACS for making AVBP available.

References

[1] T. Schuller, D. Durox, and S. Candel. Combust. and Flame, 134(1,2):21-34, 2003.

[2] D. Durox, T. Schuller, N. Noiray, and S. Candel. Proceedings of the Combustion Institute, 32(1):1391-1398, 2009.

[3] Preetham, H. Santosh, and T. Lieuwen. Journal of Propulsion Power, 24(6):1390-1402, 2008.

[4] J. H. Cho and T. C. Lieuwen. Combust. and Flame, 140(1-2):116-129, 2005.

[5] Shreekrishna, Santosh Hemchandra, and Tim Lieuwen. Combustion Theory and Modelling, 14(5):681-714, 2010.

[6] A.L. Birbaud, S. Ducruix, D. Durox, and S. Candel. Combustion and Flame,154:356-367, 2008.

[7] K. C. Schadow, E. J. Gutmark, T. P. Parr, D. M. Parr, K. J. Wilson, and J. E. Crump. Combust. Sci. and Techn., 64:167-186, 1989.

[8] T. Sattelmayer. Transactions of the ASME, J. of Engineering for Gas Turbines and Power, 125(1):11-19, 2003.

[9] C. Hirsch, D. Fanaca, P. Reddy, W. Polifke, and T. Sattelmayer. In Intl Gas Turbine and Aeroengine Congress and Exposition, number ASME GT2005-68195, 2005.

[10] T. Komarek and W. Polifke. J. Eng. Gas Turbines Power, 132(6):061503-1,7, June 2010.

[11] Palies P., Durox D., Schuller T., and Candel S. Combustion and Flame, 2010.

[12] A. Huber and W. Polifke. Int. J. of Spray and Combustion Dynamics, 1(2):199-229, 2009.

[13] A. Huber and W. Polifke. Int. J. of Spray and Combustion Dynamics, 1(2):229-250, 2009.

[14] A. Ulhaq, S. Hemchandra, L. Tay-Wo-Chong, and W. Polifke. In 19th International Congress on Sound and Vibration (ICSV19), Vilnius, Lithuania, 2012.

[15] J. Legier, T. Poinsot, and D Veynante. Proceedings of the Summer Program, Center for Turbulence Research, Stanford University pages 157-168, 2000.

[16] B. Franzelli, E. Riber, L.Y.m. Giquel, and T. Poinsot. Combustion and Flame, 159:pp. 621-637, 2012.

[17] K.T. Kim, J.G. Lee, B.D Quay, and D.A Santavicca. Combustion and Flame, 157:1731-1744, 2010.

[18] T. Poinsot and S. K. Lele. J. of Comput. Phys., 101(1):104-129, 1992.

[19] L. Tay Wo Chong, S. Bomberg, Ulhaq A., T. Komarek, and W. Polifke. In Proceedings of ASME Turbo Expo 2011, number GT2011-46342, Vancouver, Canada, 2011.

[20] Kyu Tae Kim, Jong Guen Lee, Bryan D. Quay, and Domenic A. Santavicca. Combustion Science and Technology, 183(2):122-137, 2011.

[21] W. Polifke and C. J. Lawn. Combust. Flame, 151:437-451, 2007.