FLAME DESCRIBING FUNCTION CALCULATIONS OF A TURBULENT PARTIALLY-PREMIXED FLAME FROM LES

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The present work deals determines of the non-linear heat release response to acoustic forcing of a partially-premixed turbulent flame (known as a Flame Describing Function (FDF)) from high-fidelity Large Eddy Simulations (LES). The target case is a bluff body stabilised partially-premixed turbulent flame, for which experimental measurements have been carried out. The simulations are performed using a low-Mach number solver of the open source CFD toolbox, OpenFOAM, with the combustion modelled using the Partially Stirred Reactor (PaSR) combustion model combining a global one-step chemical reaction mechanism. The unforced/forced reactive flows are simulated in order to validate the computational code. The simulations capture the unforced flow fields, the flame dynamics and the response of the flame to harmonic excitation with good accuracy. On this basis, harmonic acoustic forcing is imposed as a hydrodynamic velocity fluctuation at the inlet whose forcing amplitude and frequency can be varied independently. By extracting the gain and phase shift of the heat release rate response to harmonic forcing in velocity, we obtain the full FDF. The nonlinearity of the obtained FDF is clearly observed which is of importance to the appearance of limit cycle phenomena. The work thus confirms that low-Mach number LES, in this case via the open source OpenFOAM, provides a useful tool for characterising the non-linear response of lean partially-premixed turbulent flames to acoustic forcing.

1. Introduction

One serious issue related to lean combustion for modern low NO_x gas turbines is damaging combustion instabilities. These instabilities generally refer to sustained pressure oscillations in the combustion chamber, resulting from the coupling of the system acoustics and the unsteady heat release from the flame [1].

From numerical analysis point of view, there are two main methods for predicting combustion instability. The first is the direct method, where acoustic waves and unsteady heat release from flames are calculated simultaneously by complete 3D compressible Computational Fluid Dynamics (CFD) simulations [2]. This means that the entire acoustic system (including the whole combustor and attached components) will be calculated, which, although possible, make it impractical as an industry analysis tool. The second is the indirect method, where the acoustic wave and unsteady heat release calculations are decoupled. The response of unsteady heat release to perturbations is modelled via a flame model [3]. The acoustic waves are captured by network wave-based linear models [4] or a Helmholtz solver [5] with the obtained flame model. The present study belongs to the second group.
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Traditional flame modelling by linear Flame Transfer Functions (FTF) is restricted to small perturbations and cannot account for the limit cycle oscillations [1] nor other non-linear effects. More recently, modelling the flame response to perturbations has been extended to the weakly non-linear regime, via Flame Describing Functions (FDF) [3], in the form of:

\[ F(\omega, |u'|) = \frac{Q'/\bar{Q}}{u'/\bar{u}} = G(\omega, |u'|)e^{i\phi(\omega, |u'|)} \]  

where \( Q'/\bar{Q} \) is the normalised heat release rate fluctuation and \( u'/\bar{u} \) the normalised inlet velocity perturbation impinging on the flame. This approach makes the assumption of weak non-linearity, that is, the flame response to harmonic forcing is assumed to be primarily at the same frequency as the forcing, but with a gain and phase shift which depends upon the forcing frequency and amplitude.

Several experimental studies [6, 7] have been performed to determine non-linear flame models. The data reveal that the nonlinearity of the FDF is of central importance as it describes the mechanisms leading to amplitude saturation within limit cycles [3, 6]. For numerical studies, application of high-fidelity CFD methods in order to capture the non-linear flame response has been more limited. LES is capable of capturing the unsteady fluid behaviour. The decoupled method is advantageous as computations are performed only for a small domain within the combustor to capture the flame dynamics, as the flame response is known to be governed by the hydrodynamic, rather than acoustic, field. Besides, the CFL time step limit does not need to be based on the speed of sound. Consequently, low-Mach number or incompressible LES code [8, 9] can be used to determine the FDF as the flame response is well known to be unaffected by compressibility effects. The present study uses a similar low-Mach number LES solver to study an acoustically forced partially-premixed flame to identify the full FDF, which could be implemented in low order combustor models to investigate combustion instability.

The considered case in the present study is the bluff-body stabilised flame investigated experimentally previously [6]. Limit cycle oscillations are only observed in the partially-premixed case, which is thus the present study. The objectives of the present paper are: (1) to validate simulations of the partially-premixed flame using a LES solver based on the open-source CFD toolbox, OpenFOAM; (2) to perform LES studies of the target partially-premixed flame for the first time; (3) to determine the full FDF of the case using LES for the first time.

2. Experimental setup and numerical methods

The ethylene-fuelled burner considered here is shown in Fig.1(a), which is described in detail in Ref. [6]. In the experiments, the system can be operated in externally-forced or self-excited mode under partially-premixed conditions. For FDF determination, only externally-forced conditions are considered and thus part of the system (downstream of the plenum in Fig.1(a)) is considered for the simulations. The burner consists of two concentric cylindrical ducts with the dimensions given in Fig.1(b). The fuel is injected radially through 6 injection holes along the circumference of the central pipe. It should be noted that the global equivalence ratio is \( \phi = 0.55 \) for the externally forced cases, and \( \phi = 0.61 \) for the self-excited cases. The present LES performs externally forced simulations for both the two equivalence ratios. For the externally forced cases, the acoustic forcing was generated by two loudspeakers mounted at the plenum chamber, introducing air velocity oscillation with chamber.

In the present study, large eddy simulations are performed based on the open source CFD toolbox, OpenFOAM. Specifically, a modified version of the reactingFOAM solver is used which has been applied in previous LES studies of turbulent combustion [10]. The reactive flow equations are the Favre-filtered Navier-Stokes equations of mass, momentum, species mass fraction and energy. Heat loss effects can thus be considered in the present simulations.

To close the governing equations, turbulence modelling is required. The popular Smagorinsky
LES subgrid scale model \[11\] is applied, i.e.

\[ \mu_t = \bar{\rho} (C_s \Delta)^2 |\tilde{S}| \]  

where the model constant \( C_s \) is equal to 0.167, \(|\tilde{S}|\) is the strain rate magnitude of the resolved velocity, and \( \Delta \) is the filter cutoff width. To improve the model performance near the wall, the turbulent viscosity (Eq.(2)) is damped by using the model for van Driest damping. In OpenFOAM, the damping is derived by changing the filter width, i.e.

\[ \Delta = \min(\Delta_m, \left(\frac{\kappa}{C_\Delta}\right) y_w \left(1 - e^{-y^+/A^+}\right)) \]  

where \( \Delta_m \) is the cubic root of the cell volume, \( \kappa = 0.4187 \) the von Karman constant, \( C_\Delta = 0.158 \), \( A^+ = 26 \), \( y_w \) represents the distance to the wall, and \( y^+ \) means the dimensionless distance to the wall.

For the target case, the air and fuel are not fully premixed prior to the combustor, which results in a partially-premixed flame. The present LES study applies the PaSR (Partially Stirred Reactor) model \[10\] to deal with the turbulence-combustion interactions. It solves the filtered LES equations using a model of the filtered combustion reaction rates, \( \dot{\omega}_j \) for \( j \)-th species. The reaction rate for \( i \)-th species can be scaled by the reactive volume fraction, \( \kappa \), as \[12\]:

\[ \frac{\partial C^i}{\partial t} = \frac{C^i_1 - C^i_0}{\Delta t} = \kappa RR_i(C^i_1) \]  

where the term \( RR_i \) is the laminar Arrhenius reaction source term, i.e. \( RR_i = \dot{\omega}_i(\bar{\rho}, \tilde{T}, \tilde{Y}_j) \). Correspondingly, the reactive volume fraction, \( \kappa \), is modelled as \[12\]:

\[ \kappa = \frac{\tau_c}{\tau_c + \tau_m} \]  

where \( \tau_m \) is the turbulent mixing time scale and \( \tau_c \) the reaction time scale calculated by solving the fully coupled ODEs for the reaction system.

The reaction time scale \( \tau_c \) is determined by the chemical mechanisms. For the present ethylene/Air reaction system, the global one-step (5 species) mechanism by Westbrook and Dryer \[13\] is applied. For the turbulent mixing time, \( \tau_m \), a recently developed model is used \[10\]:

\[ \tau_m = c_m \sqrt{\tau_\Delta \tau_K} \]

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**Figure 1**: (a) Schematic of the experimental test case for partially-premixed combustion \[6\]; (b) computational setup showing for the present LES studies a cut \((z = 0)\) of the computational domain.
where the subgrid time scale $\tau_{\Delta}$ and Kolmogorov time scale are calculated by:

$$
\tau_{\Delta} = \frac{\Delta}{u'} = \frac{\Delta}{\sqrt{2k/3}}; \quad \tau_K = \left(\frac{\nu}{\varepsilon}\right)^{1/2}
$$

with $\Delta$ the cell scale, $k$ the subgrid turbulent kinetic energy, $\varepsilon$ the subgrid dissipation rate and $\nu$ the laminar kinematic viscosity. A value of 0.5 is used for the model constant $c_m$ based on tests of simulation experiments.

The turbulent mixing model shown in Eq.(6) was implemented in OpenFOAM toolbox (version 2.3.0). The algorithm for pressure-velocity coupling is based on the PIMPLE method. The convection divergence terms are discretised using a second order central difference scheme with the Sweby flux limiter to avoid unphysical oscillations. For temporal advancement, the second order implicit Crank-Nicolson scheme is used to discretise the unsteady terms, coupled with a fraction of the first-order implicit Euler scheme to stabilise the calculations.

A $z-$cut of the computational domain is shown in Fig. 1(b) including the coordinate system. An unstructured mesh is used containing about 3.48 million cells. The time-averaged bulk velocity at the combustor inlet is $V_b = 9.9 m/s$, giving a Reynolds number of $Re = dV_b/\nu = 17000$. To emulate the acoustic forcing, a single frequency harmonic velocity is superimposed on the mean flow, as:

$$
V = V_0 \left[1 + A \sin(2\pi ft)\right]
$$

where $V_0 = 5.17 \text{ m/s}$, $A$ is the velocity forcing amplitude and $f$ the forcing frequency. $A$ and $f$ are varied independently in the simulations in order to obtain the FDF. This form for the forcing has been used to simulate harmonic loudspeaker forcing of a flame in previous numerical studies [8, 9].

In the simulations, a lower temperature than the adiabatic temperature ($T_{ad}$ is around 1710\text{K} with equivalence ratio of 0.55) is imposed on the walls to account for the heat loss, i.e. $T_{w1} = 1500\text{K}$, $T_{w2} = 800\text{K}$ and $T_{w3} = 1000\text{K}$ in Fig. 1(b). All the other walls are adiabatic. To determine the FDF defined in Eq.(4), the phase of the recorded velocity signal at point $P_0$ during the simulations is used as the phase of the reference velocity.

Figure 2: Time-averaged results of the unforced reactive flow. The heat release rate in watt (W) from the present LES (left) and the FSD image from the experiment [6] (right), at a $z$-cut of $z = 0$.

### 3. Validation of the computational code

The reactive flows without/with acoustic forcing are simulated to validate the computational code. The natural flow in the absence of acoustic forcing is firstly studied. Figure 2 shows the time-averaged heat release rate from the present LES calculation and the Flame Surface Density (FSD) image from experimental measurements [6], which represents a qualitative comparison of the heat release of the unforced reactive flow. The agreement of the numerical prediction and the experimental data is reasonable. It seems that the present LES gives a slightly longer flame compared with the experiments, which implies that the speed of the combustion process is slightly under-estimated by LES. The combustion appears a little too strong in the present LES near the shear layers along the side recirculation zones, even though low temperatures are imposed on the walls to account for the heat loss.
Snapshots of the unforced reactive flow fields are shown in Figs. 3 and 4 for different flow quantities, including axial velocity ($V$ in m/s), temperature ($T$ in K) and mass fraction of fuel ethylene ($Y_{C_2H_4}$), at different locations. It can be observed that the flame is anchored at the shear layers from the wake of the bluff body and the side recirculation zones. Due to the intense heat release, the main central recirculation region behind the bluff body is enlarged. Figures 3(c) and 4 show the mass fraction flow fields of the fuel ethylene. Note that a mass fraction of 0.036 of fuel ethylene produces a global equivalence ratio of $\phi = 0.55$ under the fully premixed conditions. The results in Fig. 3(c) demonstrate that the fuel is mixed with the incoming air after the injection holes. Prior to the combustor inlet, the fuel and the air are not fully premixed. This can be seen more clearly in Fig. 4. The fuel is spatially distributed and evolves with the main flow to the downstream region.

Figure 3: Snapshots of the unforced reactive flow field from the present LES calculation: (a) axial velocity $V$ (m/s); (b) temperature $T$ (K); (c) mass fraction of the fuel ethylene, at a $z$-cut of $z = 0$.

Figure 4: Snapshots of the mass fraction of fuel ($Y_{C_2H_4}$) for the unforced reactive flow at different distances from the bluff body ($y$-cut): (a) $y/d = 0.5$; (b) $y/d = 1.0$; (c) $y/d = 2.0$; (d) $y/d = 2.5$.

The forced reactive flow case is simulated to evaluate the performance of determining the heat release response. It is accomplished by imposing the velocity fluctuations on the mean velocity at the computation inlet (see Eq. (8)) with a forcing frequency of $f = 160$ Hz.

Fourier Transforms are used to process the time series of the heat release rate and the reference velocity. The normalised amplitude of the heat release rate fluctuation as a function of the forcing amplitude $A$ is shown in Fig. 5 including the experimental measurements. The present LES predictions agree with the experimental measurements very well for both gain and phase.

The response amplitude in Fig. 5(a) demonstrates that the response is nearly linear up to the forcing amplitude of around $A = 0.35$ and then non-linear effects start to appear. The present LES calculation predicts the transition from linear to non-linear takes place slightly earlier than that in the experiments. The phase results in Fig. 5(b) show a slight increase with forcing amplitude, which is captured well by the present LES. The flame dynamics at a high forcing amplitude of $A = 0.65$ and a forcing frequency of $f = 160$ Hz are visually shown in Fig. 6 at every $60^\circ$ phase angle, for
Figure 5: (a) Dependence of the amplitude of the heat release rate response with velocity fluctuation amplitude $A$; (b) the dependence of the phase of the heat release rate response $\varphi$ (Eq. (1)), at forcing frequency $f = 160\,\text{Hz}$. Experimental data are from [6].

both the LES predictions and the experimental measurements. The image sequence shows clearly the deformation of the flame base later resulting in rollup of the flame front stabilised at the inner shear layer radially inward and the outer layer radially outward, which is similar to that in the fully premixed flame case [6, 8]. It seems that the decrease of the old mushroom-shaped vortex occurs slightly later in the present LES than that in the experiments, implying that the combustion process is slightly under-estimated in the LES. It was observed in the experiments that the flame can impinge on the wall (see Fig. 6(d)) during the process. The wall-flame interactions are not captured well by the present LES. We thus concludes that the unsteady flame behaviour is generally well captured by the LES, with both the combustion mechanism and heat loss effects playing an important role.

Figure 6: Comparisons of the mean heat release rate (in $W$) from the present LES (left) and phase-averaged FSD image from experiment [6] (right) at different phase angle with strong acoustic forcing: $f = 160\,\text{Hz}$ and $A = 0.65$.

4. Full FDF determination by the present LES

The previous section confirms that the present LES code based on OpenFOAM toolbox can capture the reactive flow field well and the unsteady heat release with acoustic forcing can also be predicted with good accuracy. The simulation target case now turns to the self-excited set of experiments in Ref. [6], in which the equivalence ratio is $\phi = 0.61$ and no experimental data regarding the FDF is available. The same numerical method is applied to that in the previous section, except that the equivalence ratio is $\phi = 0.61$ instead of $\phi = 0.55$. In the LES, the frequencies range from 150 Hz to 600 Hz, as the self-excited oscillation was observed to occur around $f = 348$ Hz in the experiments [6]. For each frequency, four forcing amplitudes are performed, $A = 0.1, 0.2, 0.3$ and 0.4.
The dependence of the flame response on the forcing amplitude is shown in Figs. (7a)-(7b). The heat release saturates for all the forcing frequencies except the lowest frequency at \( f = 150 \) Hz. The results indicate that the amplitude of the heat release response doesn’t change significantly for all the forcing amplitudes (\( A \geq 0.1 \)) presented here, for frequencies \( f \geq 250 \) Hz. For the phase results shown in Fig. (7b), it can be observed that the phase is nearly constant across the four forcing amplitudes for the forcing frequencies of \( f = 150 \) Hz and \( f = 250 \) Hz. At frequencies of \( f = 300 \) Hz and above, large phase changes are observed with forcing amplitude. With forcing frequency of \( f = 350 \) Hz, the phase result jumps from around \(-0.67\pi\) with a forcing amplitude of \( A = 0.1 \) to around \(-0.18\pi\) with \( A = 0.2 \), giving a phase change of around \(0.49\pi\). This large phase change may contribute to the limit cycle state of the oscillations.

The corresponding FDF from the present LES is given in Fig. (7c). This will to be used to analyse the combustion instability of the system by incorporating into the low order network model described in Ref. [4]. All the 24 LES runs use the same time step of \( \Delta t = 4.34 \times 10^{-6} \) s. The total CPU time used for the full FDF is around 12900 h. It can be seen that the gain falls off with increasing the forcing frequency, and a small peak appears at around \( f = 300 \) Hz with forcing amplitude of \( A = 0.4 \) and at around \( f = 350 \) Hz for the other three forcing amplitudes. With increasing the forcing amplitude, the gain generally decreases. The nonlinearity of the gain is clearly evident - a linear response would not vary with forcing amplitude. For the phase response, it implies that a nearly constant time delay exists up to the frequency of around \( f = 300 \) Hz for all the forcing amplitudes and even up to \( f = 400 \) Hz with the low forcing amplitude of \( A = 0.1 \). With higher forcing frequencies of \( f > 300 \) Hz, large phase changes can be observed as already shown in Fig. (7b).

5. Conclusions

Large Eddy Simulation was used to determine the non-linear heat release response to acoustic forcing, i.e. the FDF, based on the open source CFD toolbox OpenFOAM. The target case is a bluff-body stabilised, lean partially-premixed flame combustor developed at Cambridge University, for which previous experimental data are available. This is the first work, to the authors’ knowledge, which studies this particular flame using LES and determines the full FDF from LES.

The LES method based on the CFD toolbox OpenFOAM was firstly validated. The turbulent combustion was modelled using the Partial Stirred Reactor (PaSR) model with a global one-step reaction mechanism. Both unforced and forced reactive flow were carried out and compared with available experimental data. The results demonstrate that both the flow and flame dynamics, as well as the unsteady heat release, were captured well. Based on that, the simulations were then performed with varying the inlet velocity in order to determine the full FDF. Both the forcing frequency and the forcing amplitude were varied independently. Six frequencies were studied with four normalised
forcing amplitudes for each frequency. The nonlinearity of the obtained FDF was clearly observed. Heat release saturation and phase changes were also observed at high forcing frequencies of around $f \geq 300$ Hz, which could contribute to the limit cycle of the combustion instability.

This work confirms that open-source LES software, OpenFOAM, can be used to study lean partially-premixed combustion problems numerically, and good accuracy can be obtained. The study also suggests that a sufficiently accurate flame model can be deduced from the high-fidelity LES calculations based on the CFD toolbox OpenFOAM.

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