Large Eddy Simulation of an Oscillating Flame in Turbulent Flow around a Bluff Body

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Abstract

The present research aims at providing a reliable model for the simulation of oscillating flames which are often discovered in industrial gas turbine combustors operating at lean premixed conditions. The paper presents a Large Eddy Simulation of an oscillating bluff-body stabilised flame with a probability density function model of the subfilter scale interaction. The results show good overall agreement with the measurements, especially with regard to the phase-resolved spatial extent of the reaction zone. A phase shift between the computed total heat release rate and the measured hydroxyl chemiluminescence is observed. The mass fraction of formaldehyde determined in the median plane of the combustion chamber has been identified as a useful measure for the total heat release rate.

1 Introduction

Due to the necessity of complying with stringent emission standards, manufacturers of gas turbine combustors are required to resort to lean burn technologies. Yet gas turbine combustors that operate at lean premixed or partially premixed conditions are often prone to self-induced flame oscillation, which causes excessive wear of components of the combustor and significant reduction in the energy efficiency. Therefore manufacturers of gas turbine combustors are keen to predict oscillating flames already at the design stage.

The phenomenon of oscillating flame appears as the result of a complex interaction between the zone in which chemical reactions proceed (reaction zone) and the stress field. During the past three decades the problem of self-induced flame oscillation has been at the centre of the researchers’ attention, but to date the coupling between the reaction zone and the stress field is not yet fully understood. The prediction of oscillating flames in industrial gas turbine combustors necessitates efficient and accurate solvers for turbulent flows. Large Eddy Simulation (LES) is such a flow solver which strikes a balance between both efficiency and accuracy. When applied to reacting mixtures LES requires modelling of the interaction between hydrodynamic and constitutive mass fraction fields on length scales which are not resolved numerically. A Probability Density Function (PDF) model, which accounts for this subfilter scale interaction, yielded good agreement with measurements in a variety of flows, see for example Jones and Navarro-Martinez (2009) and Jones and Prasad (2010). Additionally, the constitutive model for the reaction rates plays an important part in the prediction of oscillating flames.

The aim of the present research is to provide a modelling framework for the simulation of oscillating flames in turbulent flow. It is demonstrated that LES with a PDF model of the subfilter scale interaction and a detailed reaction mechanism is able to reproduce the characteristic properties an oscillating flame in an industrially relevant gas turbine combustor. This is supplemented by a discussion of useful measures for quantifying the variation of the total rate of generation of heat by reaction (total heat release rate) in the oscillating flame. The configuration chosen for study consists of a cone-shaped bluff body, which is hold in place by a rod in a cylindrical combustion chamber. The flow of a reacting mixture around a bluff body is often encountered in industrial gas turbine combustors. In such a flow the reaction zone appears in the shear layers downstream of the obstacle which passively maintains the position of the high temperature region away from the walls of the combustion chamber.

In the first part of the paper, details on the experiment and modelling approach are given. The second part of the paper is concerned with assessing the results of the simulation by comparison with the measurements. In addition, various indicators for determining the variation of the total heat release rate in the oscillating flame are examined.

2 Experiments

The experiment to be investigated in the present work has been developed by Balachandran (2005). In this experiment the flame was caused to oscillate by use of loudspeakers which excite harmonically the mass flow rate of the mixture at the inlet of the combustion chamber. In comparison to self-induced flame oscillation, such a flow is easier to control as the bulk
behaviour is largely determined by two prescribed parameters; the frequency and amplitude of the mass flow rate variation. The flame response has been quantified by different measurement techniques for several frequencies and amplitudes of the excitation signal. Measurements on the velocity response of a non-reacting air flow to harmonic excitation of the mass flow rate in this same apparatus have been obtained in an experiment by Ayache et al. (2010).

Figure 1 displays a simplified diagram of Balachandran’s apparatus to determine the flame response to harmonic excitation of the mass flow rate. In operation a lean premixed mixture of ethylene, C\textsubscript{2}H\textsubscript{4}, and air at an equivalence ratio of 0.55 has been injected through a supply unit into the bottom section of the apparatus. The mean mass flow rate through the plenum chamber has been adjusted to yield a bulk-averaged axial velocity \(v_0\) of 10 m/s at the inlet of the combustion chamber. The bluff body base diameter, \(D_b\), with a value of 25 mm serves here as a reference dimension. At the outlet, the chamber is open to the atmosphere. The length and diameter of the combustion chamber are 3.2 \(D_b\) and 2.8 \(D_b\), respectively. The excitation of the mass flow rate using the loudspeakers is approximately sinusoidal with amplitude \(A\), and frequency \(f\). By measuring the flow response to variation of these parameters the Flame Transfer Function (FTF) was determined. However, in the study presented only one parameter set, \(A = 0.64 \times v_0\) and \(f = 160\) Hz, is considered.

![Diagram of Balachandran's apparatus](image)

Figure 1: Diagram of Balachandran’s apparatus for determining the fluorescence of molecular species in the oscillating flame (not to scale); 1: ethylene-air injection, 2: plenum chamber, 3: slow straightener, 4: loudspeaker, 5: laser, 6: bluff body with holder, 7: camera, 8: quartz tube.

Among the different measurement techniques for determining the heat release rate are the detection of chemiluminescence from chemically excited hydroxyl radical, OH\(^*\), and laser induced fluorescence emitted from OH, where the asterisk refers to the chemically excited state. The signals have been detected in a plane parallel to the median plane of the combustor. Another measure for the heat release rate variation is computed directly from the raw images of the OH fluorescence, namely the Flame Surface Density (FSD). An additional measure being relevant in this report is the mass fraction of formyl radical, HCO. In turbulent flows the mass fraction of HCO is experimentally determined through estimating the forward reaction rate of the reaction forming the greater part of HCO, which is

\[
\text{CH}_2\text{O} + \text{OH} \rightarrow \text{HCO} + \text{H}_2\text{O}.
\]

The forward reaction rate of Eq. (1) is proportional to the product of the mass fractions of formaldehyde, \(\text{CH}_2\text{O}\), and \(\text{OH}\). By detecting the laser induced fluorescence emitted from \(\text{CH}_2\text{O}\) simultaneously with \(\text{OH}\) fluorescence, the product of the mass fractions is approximated by the product of the two fluorescence intensity signals. This indicator is subsequently referred to as heat release rate imaging (HR). For further information on alternative methods the reader is referred to Balachandran (2005) and Ayoola (2005). It is important to note that the scale of the fluorescence or chemiluminescence images is arbitrary so that suitable scaling is required. In this experiment all the measures for the heat release rate were scaled by means of the time and spatial average of the intensity. To characterise the periodic evolution of the heat release rate, phase-averaging with respect to the excitation signal has been carried out. The notation \(\langle \cdot \rangle\), \(\langle \cdot \rangle\) and \(\langle \cdot \rangle\) is introduced to distinguish between time, spatial and phase average, respectively.

In the experiment of Ayache et al. (2010) the response of the velocity field to excitation of the mass flow rate was measured. The medium was air. Excitation of the mass flow rate has been achieved in just the same way. Ayache et al. focussed on only a few parameter sets among which is \(A = 0.60 \times v_0\) and \(f = 160\) Hz. The measurements comprise profiles of the phase-averaged axial velocity component at several positions in the median plane of the combustion chamber.

3 Modelling

The experiment of Ayache et al. is simulated first to assess the mesh resolution and the placement of the boundaries in the computational domain. With the model established in course of the first simulation, the experiment on oscillating flames is then simulated. The computational domain for the simulation along with the boundary conditions are presented in Figure 2. The domain is discretised with \(2.19 \times 10^6\) control volumes which are clustered around the bluff body and the inlet of the combustion chamber. A turbulent velocity field has been prescribed at the inlet of the computational domain. This velocity field has been computed by use of the synthetic turbulence gen-
eration method of Klein et al. (2003). In the simulation of both the non-reacting and reacting mixture a sinusoid with the frequency $160 \text{ Hz}$ and the amplitude $0.6 \nu_b$ has been superimposed onto the turbulent inlet velocity field. The experimental results have shown no significant alteration of the flame response when the amplitude of the excitation signal has been increased to yield values greater than $0.6 \nu_b$ for the axial velocity component at the inlet of the combustion chamber. This allows the comparison of the flow field response of air with that of the reacting mixture and also the predicted flame response with the experimental results for $A = 0.64 \nu_b$. The mixture of $\text{C}_2\text{H}_4$ and air is premixed prior to injection into the plenum chamber therefore the mass fractions are assumed to be homogenous across the inlet plane. The temperature at the inlet is $293 \text{ K}$. It is assumed that the flux of heat at the inner surface of the walls of the combustion chamber is zero as it is generally small compared to the heat release rate. The fluid being entrained by the jet at the exit of the combustion chamber is in both simulations represented by an air co-flow at a temperature of $293 \text{ K}$. This co-flowing stream was not present in the experiment but was included to avoid large unphysical recirculation zones in the outer region. The axial co-flow velocity was chosen such that the time-averaged mass flow rate is $10\%$ of the mass flow rate at the outlet of the combustion chamber.

The LES flow solver is block-structured and uses second-order discretisation schemes. In both simulations the computational time step was chosen to be $5.0 \times 10^{-6} \text{s}$. The subfilter stress is approximated by the dynamic Smagorinsky model. In the differential equations describing the evolution of the PDFs the unknown transport and mixing term are approximated by the Smagorinsky subfilter viscosity model and the Linear Mean Square Estimation (LMSE) closure, respectively. The PDF differential equations are solved using the Eulerian stochastic field method with an Ito interpretation of the stochastic integral. In the present case, the simulation of the oscillating flame has been carried out using four stochastic fields. For a more detailed account on the PDF approach, the reader should consult Sabel’nikov and Soulard (2005). The reaction rates are modelled by using the reduced reaction mechanism of Luo et al. (2012). This mechanism involves 22 molecular species and 18 global reactions and has been obtained by systematic reduction of a detailed mechanism which comprised 75 species and 529 reactions, see Wang and Laskin (2000).

## 4 Results and discussion

### Air flow

A phase-averaged streamline pattern is displayed in Figure 5. It can be seen that recirculating flow establishes downstream of the the conical bluff body (central recirculation zone) and in proximity to the cylindrical wall of the combustion chamber (outer recirculation zone).

<table>
<thead>
<tr>
<th>Name</th>
<th>P1</th>
<th>P2</th>
<th>P3</th>
<th>P4</th>
<th>P5</th>
<th>P6</th>
</tr>
</thead>
<tbody>
<tr>
<td>x/D_b</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>r/D_b</td>
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<td>0.6</td>
<td>1.2</td>
<td>0.0</td>
<td>0.6</td>
<td>1.2</td>
</tr>
</tbody>
</table>

### Table 1: Probe positions

![Figure 2: Sketch of the computational domain and boundary conditions for the simulation (not to scale).](image)

The boundary conditions are as follows: 1: air inlet/ethylene-air inlet, 2: air co-flow, 3: free slip boundary, 4: zero-gradient outlet, 5: no-slip walls.

Figure 3: Profiles of the phase-averaged axial velocity; symbols: experimental data of Ayache et al. (2010), solid lines: simulation, dashed line: excitation signal.
Shear layers are formed between the central recirculation zone and the annular jet and between the annular jet and the outer recirculation zone. Table 1 lists the probe positions at which the axial velocity component has been measured. They are placed in each of the characteristic zones of the flow. Figure 3 compares the measured and predicted phase-averaged axial velocity component at these six probe locations. The scaled phase with respect to the excitation signal is therein denoted by $\gamma$. Generally, the predicted solutions compare well with the measurements at all positions. It is worth noting that good agreement is obtained at P2, which is the position closest to the inlet of the computational domain and therefore an indicator for the adequacy of the imposed velocity field. At P5 and P6 the axial velocity is underpredicted but the shape is reproduced satisfactorily. Two more parameter sets, $A = 0.89 v_b$ and $f = 50$ Hz, and $A = 0.75 v_b$ and $f = 320$ Hz for which experimental data was made available have been simulated to validate the model against measurements.

The predicted results are not displayed here but showed also good agreement with measurements throughout, in particular at P5 and P6. At P1 and P3, which are probe positions in the central and outer recirculation zone, the axial velocity varies much less with $\gamma$ in comparison to the position in the annular jet (P2). From the streamline pattern in Figure 5 it becomes clear that both the central and outer recirculation zone are excited at the frequency of the oscillating annular jet. However, the recirculation zones are displaced only marginally along the center axis which implies a small variation of the axial velocity about the time average. It has been further observed in the streamline pattern that the outer recirculation zone extends axially across the outlet of the combustion chamber which complicates the imposition of boundary conditions there. This thus supports the approach taken here. Figure 4 shows a comparison between the measured and predicted phase-averaged fluctuations of the axial velocity. The agreement is less satisfactory than in the previous comparison. At P1-P3 discrepancies between the predicted and measured profiles are found. The streamline pattern (Figure 5) reveals that the shear layers between the radially widened annular jet and the recirculation zones are passing periodically through the probe positions. These events may lead to intermittency to which the dynamic Smagorinsky model is prone and this is most likely to have greater impact on the prediction of the turbulent fluctuations, see da Silva (2009). Further downstream, at P4-P6, the measured profiles are overall better predicted. The results presented in this section are considered reliable indicators that the domain discretisation and the placement and modelling of the boundary conditions is adequate.

**Oscillating flame**

First, the general features of the oscillating flame are described and contrasted with the predicted velocity field in the oscillating air flow. The oscillating flame together with the corresponding streamline pattern is depicted in Figure 5. The flame contour is evaluated from the heat release rate field for a value of 5 % of the maximum heat release rate. It must be acknowledged that variation of the contour value affected slightly the contour shape at the downstream end as the gradient of the heat release rate is smaller there than it is in the shear layers between the annular jet and the recirculation zones. However, the criterion suffices to explain the main features of the flow. It can be seen that the flame elongates in axial direction along the annular jet and becomes thinner in the cross direction for increasing $\gamma$. In fact, towards the end of the period, $\gamma > \frac{3}{4}$ (not shown here), the deformation leads to a break up of the flame. It has been verified that this is not an artifact of the flame contour visualisation. Beyond break up, the upstream part propagates upstream towards the inlet of the combustion chamber, while the downstream part extinguishes when propagating further downstream. The phase at which the break up occurs is $\gamma \approx 0.85$, and does not coincide.

![Figure 4: Profiles of the phase-averaged fluctuations of the axial velocity: symbols: experimental data of Ayache et al. (2010), solid lines: simulation, dashed line: excitation signal.](image-url)
with the occurrence of the maximum total heat release rate, which is at $\gamma \approx 0.63$. It is observed that the presence of the central and outer recirculation zones leads additionally to a deformation of the flame in the radial direction. This forms a mushroom-like structure at the downstream end of the flame, which can be observed at $\gamma = \frac{1}{3}$. In comparison to the non-reacting case, both the center and outer recirculation zones suffer more pronounced deformation along the center axis. A general feature of the flame appears to be that the thickness of the reaction zone varies noticeably along the mean path of the reaction zone. At $\gamma = \frac{1}{3}$, for instance, the maximum thickness is found at the downstream end of the flame and is approximately three times larger than the minimum thickness, which is in the shear layers. The ratio becomes even larger for $\gamma > \frac{1}{3}$. In theoretical work on premixed oscillating flames it is usually assumed that the flame is a singular surface with respect to certain field variables, such as temperature and density. It remains unclear whether models based on such assumptions can be used to explain the break up phenomenon, which resembles not least a local “necking” of the reaction zone with finite thickness. Based on the above results it is highly questionable that the flame can be conceived of as a discontinuity, especially with regard to devising jump conditions for the field variables.

The predicted reaction zone will now be assessed in more detail by comparison with experimental data. As was mentioned in Section 2, the heat release rate is quantified experimentally only implicitly through intensity signals emitted from excited molecular species, which are known to correlate well with the heat release rate. A comparison between experiment and simulation can therefore only be sensible if the data obtained from the experiment as well as the simulation are scaled in the same way. In the first part of this discussion the spatial extent of the reaction zone is analysed. The second part focuses on measures to quantify the periodic evolution of the total heat release rate.

The contour of the reaction zone is compared with experimental data in Figure 6. The data obtained from the simulation has been scaled with the time and spatial average of the heat release rate in the median plane of the combustion chamber. All contours have the same value. Both FSD and HR are measurement techniques which have been developed specifically for determining the spatial extent of the reaction zone. Despite scatter in the experimental data the comparison can serve to identify potential deviations between experiment and simulation, such as observed at $\gamma = \frac{2}{3}$. The predicted reaction zone appears deflected towards the center axis, whereas both experimental results suggest that the reaction zone reattaches at the wall of the combustion chamber. A plausible explanation for this deflection relates to the modelling assumption that the flux of heat at the inner surface of the combustor wall is zero. The flux of heat is proportional to the temperature difference between the wall and the gas, hence becoming large when the reaction zone approaches the wall of the combustion chamber. This thus requires the heat transfer at the inner surface, heat conduction in the wall and the heat transfer at the outer surface of the wall to be taken into account. The deflection of the reaction zone predicted in the simulation may be the sole cause of the break up of the flame observed. No such phenomenon has been reported in the experimental work of either Balachandran (2005) or Ayoola (2005). The best agreement between experiment and simulation is achieved at a phase value of $\gamma = \frac{1}{4}$ when the reaction zone is freely propagating and not suffering effects from the presence of the combustor
wall. However, the HR result suggests that the reaction zones extends further towards the center axis, which is not observed in the FSD result. In the simulation, the total heat release rate, $Q_{tot}$, is evaluated as the integral over the volume of the combustion chamber; its time average being $\langle \frac{Q_{tot}}{\gamma} \rangle = 6.1$ kW. The scaled total heat release rate variation obtained from the simulation together with experimental data is shown in Figure 7.

![Figure 6: Contour of the reaction zone; dark grey line: FSD data of Balachandran (2005), light grey line: HR data of Ayoola (2005), black line: simulation.](image)

Figure 6: Contour of the reaction zone; dark grey line: FSD data of Balachandran (2005), light grey line: HR data of Ayoola (2005), black line: simulation.

Note that the total emission intensity of OH\* is simply the integral over the plane in which the measurements have been recorded. The predicted heat release rate varies approximately 50% about the time-average mean value. It can be seen that a phase shift of $\Delta \gamma \approx 0.2$ occurs between the predicted heat release rate variation and the measured OH\* chemiluminescence. The corresponding time shift for the investigated excitation frequency equals approximately 1.3 ms. Chemiluminescence of OH\* is frequently used as a measure for the total heat release rate variation as the emission intensity, $I$, has been found to scale linearly with the fuel consumption rate. It originates from a radiative transition of the molecular species in the excited state to the ground state. Besides spontaneous emission, the ground state of the excited molecule can be attained by quenching. In fact, the rate of spontaneous emission for OH\* is given by the Einstein A coefficient $1.4 \times 10^9$ s$^{-1}$, which is orders of magnitude smaller than the reaction rates associated with quenching; typically of the order of $10^{12}$ s$^{-1}$, see Hidaka (1982). Hence, quenching is dominating the transition from the excited state to the ground state. The mass fraction of OH in the ground state is thus merely proportional to the OH\* chemiluminescence. Although the formation and decay of OH\* has not been included in the present reaction mechanism the predicted OH (ground state) mass fraction can serve to verify the phase shift observed between $Q_{tot}$ and the measured OH\* chemiluminescence. It is of importance to note that chemiluminescence is a line-of-sight integration and contains therefore intensity contributions of the three-dimensional emission field. This has been mimicked in the present case by performing the line-of-sight integration of Ruder et al. (1989) of the predicted three-dimensional OH mass fraction field. The integral value over the obtained intensity image as a function of phase is plotted in Figure 7. It can be seen that the prediction has the same phase shift with respect to $Q_{tot}$ as the measured OH\* emission intensity. A possible explanation is that the reaction rate associated with the formation of OH is small in comparison to the reaction rates having high exothermic fractional influence on the heat release rate. For this to be concluded a detailed reaction rate balance must be performed, which has not been done in the present case. Further research is therefore required to identify the origin of the observed phase shift. It should also be investigated if the phase shift is dependent on the frequency of the excitation signal as this would have implications on the evaluation of the FTF. The OH\* emission intensity suggests an approximately 15% larger maximum value than that of $Q_{tot}$. Another remark can be made with regard to the spatial variation of OH\* chemiluminescence, which is displayed in Figure 8. The comparison with the line-of-sight integration of the predicted OH mass fraction provides further evidence that the OH\* emission signal does not correlate...
well spatially with the OH mass fraction. It is thus necessary to include additional reactions in the mechanism which describe the formation of OH\(^\ast\) and its decay to the ground state by spontaneous emission and quenching if spatially resolved OH\(^\ast\) comparison with experiment were to be made. However, a characteristic feature being observed at \(\gamma = \frac{1}{3}\) in both cases is the mushroom-like deformation of the flame at the downstream end. The last aspect to be discussed refers to the identification of alternative measures for the total heat release rate variation, which are accessible by experiment. For this reason, the mass fractions of OH and CH\(_2\)O as integrated values over the median plane are compared with \(Q_{\text{tot}}\), which is shown in Figure 9.

\[
\text{CH}_3 + \text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}, \tag{2}
\]

where the species CH\(_3\), O and H are the methyl radical, atomic oxygen, and atomic hydrogen, respectively. The product of the mass fractions of OH and CH\(_2\)O, which, as discussed in Section 2, is proportional to the reaction rate of the forward reaction forming the greater part of HCO, exhibits a distinct peak at \(\gamma = 0.75\). This has been observed neither in the experiment nor in the predicted variation \(Q_{\text{tot}}\). With appropriate calibration of the fluorescence imaging it may be possible to determine by experiment the mass fraction of CH\(_2\)O quantitatively and thus implicitly the total heat release rate variation.

5 Summary

The paper presents the simulation of an oscillating flame in a turbulent flow around a bluff body by means of LES with a PDF approach for the subfilter scale interaction. The model established has been shown capable of reproducing the velocity field of an harmonically excited air flow in the first and second moments with reasonable accuracy. In addition, the simulation of the oscillating flame revealed good overall agreement with the measurements. To avoid the predicted deflection of the flame when approaching the wall of the combustion chamber it is necessary to take heat transfer effects at the wall into account. A rather surprising result is that the predicted total heat release rate variation and the measured OH\(^\ast\) emission intensity exhibit a noticeable phase shift. The origin of the phase shift could not be identified and hence remains a subject for future work. It has been found that the integrated mass fraction of formaldehyde, CH\(_2\)O, in the median plane of the combustion chamber provides a good estimate for the total heat release rate. The LES

Figure 8: Line-of-sight integration of the predicted OH mass fraction field (upper half) and measured OH\(^\ast\) chemiluminescence (lower half) in the median plane of the combustion chamber.

Figure 9: Phase-averaged and scaled bulk intensity variation obtained in the median plane of the combustion chamber.

OH mass fraction evaluated in the plane suffers again from the phase shift with respect to \(Q_{\text{tot}}\) and therefore fails to be an appropriate measure. On the other hand, the mass fraction of CH\(_2\)O appears as a reliable indicator for the total heat release rate variation both in amplitude and phase. CH\(_2\)O is an important intermediate species in hydrocarbon combustion and is formed in a reaction which has high exothermic fractional influence on the heat release rate [Ayoola (2005)]
method outlined here constitutes a good starting point for the investigation of self-induced flame oscillation.

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References


