Large Eddy Simulation of Unsteady Flame Propagation

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1. Introduction

Gas explosions often occur in presence of elements that disturb the flame propagation. The coupling of the moving flame front and the turbulent flow field induced by the local blockage enhances the flame acceleration and the subsequent overpressure. For obstacles-aggravated explosions the mechanisms driving the pressure rise are still debated, as well as the quantification of their role and weight by varying conditions and parameters.

In the last years, thanks to the progress made in the field of experimental diagnostics, highly resolved data related to the unsteady interaction between premixed flames and obstacles have been obtained in terms of flame images and speed profiles, flow field vectors and turbulence characteristics maps [1-5]. These works have enabled a basic understanding of the development details of flames propagating in small-scale explosion chambers.

On the numerical side, the adoption of CFD modeling techniques has allowed the opportunity of simulating the premixed flames propagation through obstacles taking into account the full coupling of flow, turbulence and combustion by means of both, RANS [4, 6] and Large Eddy Simulation (LES) [7, 8] approaches.

RANS modelling solves the Reynolds time- and ensemble-averaged equations, thus eliminating the chaotic fluctuations of turbulence. With LES the large-scale time-dependent eddies are resolved, while the smaller sub-grid scale effects are modelled.

By directly computing the largest turbulent structures, LES involves a computational cost that is normally orders of magnitudes higher than that for RANS calculations. However, it is able to take into account much more physics compared to RANS.

For obstacles-induced explosions, LES is particularly useful as it captures the intrinsically unsteady nature of the phenomenon and allows a better resolution of the eddies formed around the obstruction, which have a key role in generating turbulent flame acceleration and overpressure [1-3, 6, 7]. Furthermore, LES may provide more detailed information about the velocity field, the propagation velocity and structure of the flame, and the shear layers that arise during the propagation [7, 8].

In a previous work we have developed a LES-based model to simulate the unsteady propagation of stoichiometric CH₄/air premixed flame around an obstacle in a vented combustion chamber initially filled with quiescent mixture [8]. The model has been coupled to a sub-grid combustion model that takes into account the interaction between reaction rate and flow field, thus following all the flame propagation stages from laminar to fully turbulent.

The model validation has been performed by comparing the simulation results versus the detailed experimental data by Ibrahim et al. [2]. A good agreement has been found in terms of global features of flame propagation, flame speed profile along the chamber and overpressure time history.

In the present paper, these numerical results are examined with the aim at getting insight into how the coupling of fluid-flow, turbulence and combustion affects the mechanisms correlating flame structure, speed and resulting overpressure.
2. The model

The LES model adopted to simulate the unsteady propagation of stoichiometric CH\textsubscript{4}/air premixed flame around obstacles has been described in our previous work [8]. Briefly, the employed model equations were obtained by Favre-filtering the governing equations for compressible flow with premixed combustion. The turbulence closure was achieved by using the dynamic Smagorinsky model [9]. The flame surface density approach was adopted to parameterize the chemical reaction at the sub-grid scale. In particular, the flame surface density was expressed as function of the sub-grid scale flame wrinkling factor \( \Xi_{\Delta} \) (i.e., the projection of the sub-grid scale surface in the propagating direction) [10]. To take into account the coupling of unresolved turbulence and reaction rate, \( \Xi_{\Delta} \) was modelled according to Charlette et al. [10].

The experimental data by Ibrahim et al. [2] were used to validate the model [8]. We chose as test case the experiment on the propagation of stoichiometric CH\textsubscript{4}/air premixed flame in a closed-end chamber (75 mm x 150 mm x 450 mm) containing a 50 % blockage obstacle with a rectangular cross-section (40 mm x 12 mm). The obstacle was mounted at 150 mm of distance from the closed face. The chamber was initially filled with quiescent mixture ignited at the closed end center. Figure 1 shows a schematic diagram of the combustion chamber.

![Figure 1 – Schematic diagram of the explosion chamber by Ibrahim et al. [2] (not to scale).](image)

3. Results and discussion

In Figure 2 the flame speed profile is reported as computed along the axial distance from the ignition face when the flame propagates around the obstacle (\( d > 100 \) mm): the flame is observed to accelerate past the obstacle (125 \( \leq d \leq 175 \) mm), decelerate (175 \( \leq d \leq 210 \) mm) and accelerate again (210 \( \leq d \leq 260 \) mm) downstream of the obstruction.

Figure 3 shows the time history of the mean overpressure as calculated at the bottom end of the combustion chamber starting from the ignition: two well evident overpressure peaks are observed at about 37.5 and 41.6 ms.

In Figure 4 the time sequences of the computed maps of temperature (top) and vorticity vectors magnitude (down) are presented. The vorticity is the curl of the velocity vector and, then, it represents a measure of the rotation of a fluid element as it moves in the flow field.
Figure 2 – Flame speed profile as computed along the axial distance from the ignition face.

Figure 3 – Time history of the mean overpressure as computed at the bottom end of the chamber.

Figure 4 – Temperature (K) (top) and vorticity magnitude (s$^{-1}$) (down) maps as computed at different time instants after the ignition.
To allow matching the maps of Figure 4 with the corresponding spatial flame speed profile (Figure 2) and overpressure time trend (Figure 3), for each field profile the axial distance of the flame front from the ignition face is reported together with the time instants of the two overpressure peaks found.

Figure 4 (top) shows the main features of the flame propagation: the flame approaching the obstacle almost symmetrically about the chamber centerline (28 \(\leq t \leq 33\) ms); the impingement onto the obstacle with an incomplete combustion of the fuel mixture in the upstream chamber zone (32 \(\leq t \leq 33\) ms); the separation into two opposite flames passing around the obstacle (33 \(\leq t \leq 37.5\) ms); the flames reconnection downstream of the obstacle coupled to both, the flames venting towards the chamber exit and the accumulation of a small volume of unburned mixture behind the obstacle (37.5 \(\leq t \leq 43\) ms). Furthermore, the flame front has a quasi-laminar smooth structure during the propagation up to the obstacle location (Figure 4, \(t \leq 33\) ms), while it appears as a typical premixed turbulent front when the flame burns downstream of the obstacle (Figure 4, 36 \(\leq t \leq 43\) ms).

Indeed, as the flame starts to propagate it promotes a flow in the unburned mixture because the expansion of the freshly burned gases moves the surrounding gases away.

When the unburned mixture, moved ahead by the propagating flame front, reaches the obstacle, it accelerates due to the flow cross-section constriction, thus generating a “jet-like” flow around the obstacle. Consequently, a symmetrical pair of eddies is formed either side of the obstacle, as shown in Figure 4 (down) at \(t = 28\) ms. Each eddy sheds into the stagnant wake behind the obstacle, starting from the backward facing edge of the rectangle.

As the flame approaches the obstacle, the eddies grow and move towards the chamber centerline behind the obstacle (Figure 4, 28 \(\leq t \leq 33\) ms).

When the flame touches the obstacle, it follows the high momentum jetting gases that convect the flame downstream of the obstacle itself (Figure 4, \(t \geq 32\) ms).

In these conditions, a first flame acceleration occurs corresponding to the flame passage through the obstacle-wall gap (Figure 2 and Figure 4, 125 \(\leq d \leq 175\) mm, 32 \(\leq t \leq 34\) ms).

Then, the flame decelerates expanding downstream of the obstacle (Figure 2 and Figure 4, 175 \(\leq d \leq 210\) mm, 34 \(\leq t \leq 35\) ms) and soon after it accelerates again interacting with the obstacle-induced flow vortices into the wake (Figure 2 and Figure 4, 210 \(\leq d \leq 240\) mm, 35 \(\leq t \leq 36\) ms). The vortices wrinkle, corrugate and distort the flame front (Figure 4, \(t \geq 35\) ms). This causes an increase of the flame surface area that, together with the increasing turbulence level promoting the heat and mass transport towards the flame, enhances the propagation rate.

As soon as the flame accelerates past the obstacle (Figure 2 and Figure 4, \(d \geq 125\) mm, \(t \geq 32\) ms), the overpressure starts to increase significantly (Figure 3, \(t > 32\) ms). Also during the short phase of flame deceleration downstream of the obstacle (Figure 2 and Figure 4, 175 \(\leq d \leq 210\) mm, 34 \(\leq t \leq 35\) ms) the overpressure continues to increase up to reach a first peak at about 37.5 ms (Figure 3). This peak is found at the time when the two opposite flames emerging from the obstruction approach each other and start venting towards the exit (Figure 4, \(t = 37.5\) ms).

Concerning the second overpressure peak, it corresponds to the combustion of the fuel mixture trapped behind the obstacle after that the flames joint each other and exit the chamber (Figure 3 and Figure 4, \(t = 41.6\) ms).

To get insight into the nature of the computed overpressure trend of Figure 3, it is useful to divide the combustion chamber into two parts as done in Figure 1: the first part which lies from the bottom face up to the obstacle and the second one from the obstacle up to the chamber exit. Each chamber is vented: the first chamber towards the second one and this
latter towards the atmosphere.

We have calculated the time profiles of combustion and venting rates in the two chambers, in order to quantify the role of the competition between such counteracting phenomena in generating the two dominant overpressure peaks of Figure 3. The combustion rates have been evaluated as temporal derivative of the mass of gas in each portion of the chamber. The venting rates have been computed as mass flow rate at the mid-height obstacle section \((d = 0.15)\) and at the outlet channel section \((d = 0.45)\) for the first chamber and the second chamber, respectively.

In Figure 5 the time histories of the combustion rate and venting rate are reported for each chamber together with the overpressure time trend in the channel.

![Figure 5](image-url)  

*Figure 5 – Computed time histories of the combustion and venting rates in the first and second chamber of the channel.*

From Figure 5 it turns out that up to about 32 ms, when the flame is still upstream of the obstacle (i.e., in the first chamber) (Figure 4, top), the combustion chamber is efficiently vented towards the atmosphere. Combustion rate and venting rates at both, the obstacle section and the chamber exit, assume very close values. As a result, the chamber overpressure does not increase significantly (Figure 5).

Starting from \(t \approx 33\) ms the venting rate at the obstacle section decreases (Figure 5). At this time, the flame reaches the obstacle and starts to flow around it: the passage between obstacle and chamber side walls is blocked by the flame, while unburnt mixture is still present in the first chamber (Figure 4, top). Consequently, starting from \(t \approx 33\) ms the laminar combustion in the first chamber almost proceeds as in a closed vessel.

Figure 5 also shows that before the first peak \((t \approx 37.5\) ms\) combustion rate and venting rate in the second chamber follow each other: the increasing chamber pressure and the subsequent increasing pressure drop promote the flow venting towards the exit. Indeed, the burned gases produced by the obstacle-accelerated flame almost instantaneously flow out of the channel.

As a conclusion, the pressure rise related to the first peak has to be ascribed to the violent *obstacle-side combustion* acting as an *external explosion* of a simply vented configuration.
After the first peak the pressure starts to decrease since no unburnt mixture remains in the first chamber and combustion only proceeds in the second one (Figure 4 and Figure 5, $37.5 \leq t \leq 40$ ms).

When the combustion is almost complete also in the second chamber, a second overpressure peak occurs (Figure 4 and Figure 5, $t \approx 41.6$ ms) that is again the result of the coupling between combustion rate and venting rate (Figure 5).

Before this peak, the combustion rate of the mixture accumulated behind the obstacle is enhanced by the interaction of the flame with the flow vortices shedding from the edges into the obstacle wake (Figure 4 and Figure 5, $38.5 \leq t \leq 41.6$ ms). On the contrary, the venting rate decreases since the flame exits the chamber giving rise to an external combustion of the fresh gases pushed out by the propagating flame front (Figure 4 and Figure 5, $40 \leq t \leq 43$ ms).

Consequently, the turbulent combustion of the trapped reactants (over-combustion) occurs with a stopped venting, thus causing the second overpressure peak.

4. Conclusions

In the present paper a validated LES-based CFD model has been used to study the unsteady propagation of a stoichiometric CH$_4$/air premixed flame around an obstacle in a closed-end combustion chamber initially filled with a quiescent mixture. The numerical results has allowed identifying in the competition between combustion rate and venting rate that establishes in the chamber zones upstream (first chamber) and downstream (second chamber) of the obstacle, the mechanism responsible for the two overpressure peaks observed.

When the propagating flame reaches the obstacle and starts to flow around it, the passage between the obstacle and the chamber side walls is blocked, while unburnt mixture is still present upstream the obstacle. Consequently, due to the obstacle-side combustion, the laminar propagation in the first chamber almost proceeds as in a closed vessel, thus leading to the first overpressure peak. When the combustion is almost complete also in the second chamber, the flame exits the channel, giving rise to an external combustion of the fresh gases pushed out by the propagating flame front. As a result, the turbulent combustion of the reactants trapped behind the obstacle (over-combustion) occurs with a stopped venting. This causes the second overpressure peak.

5. References