Chemical Engineering Science 71 (2012) 539–551

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Large Eddy Simulation of transient premixed flame–vortex interactions in gas explosions

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ARTICLE INFO

Article history:
Received 16 March 2011
Received in revised form
14 October 2011
Accepted 21 November 2011
Available online 29 November 2011

Keywords:
Large Eddy Simulation
Gases
Combustion
Turbulence
Explosions
Safety

ABSTRACT

In this work, a Large Eddy Simulation (LES) model was used to simulate the transient premixed flame–vortex interaction, which is the key phenomenon determining dynamics and consequences of gas explosions. In particular, the effect of the grid resolution on the impact of the combustion sub-model was investigated. To this end, LES computations were run, with and without the combustion sub-model, on three non-uniform unstructured grids with cell characteristic length varying in the ranges 2–3 mm, 1–2 mm and 0.5–1 mm. Numerical predictions were compared with literature experimental data. It has been found that the amount of detail explicitly resolved on the finer grid (having a resolution of the same order of magnitude as the laminar flame thickness) is such that, even without the combustion sub-model, the LES results obtained with this grid correctly match the experimental data in both quantitative (flame speed and flow velocity) and qualitative (shape and structure of the flame front) terms.

1. Introduction

Turbulent premixed flames, steady or unsteady, are used in a range of engineering applications including boilers, furnaces, gas turbine combustors, industrial burners and spark ignition engines. Such flames are also found in gas explosions that represent a major issue for chemical and process industries.

In gas explosions, the premixed flame propagating away from an ignition source encounters obstacles along its path that, in complex plants, consist of various shapes and boundaries. The unsteady coupling of the moving flame and the flow field induced by the presence of local blockage produces vortices of different length and velocity scales ahead of the flame front. The flame–vortex interaction leads the initially laminar flame to burn through various turbulent combustion regimes, thus accelerating the flame and increasing the rate of pressure rise (Di Sarli et al., 2007a).

In order to understand and control the hazards and risks associated with gas explosions, predictive Computational Fluid Dynamics (CFD) models are needed (Di Benedetto and Di Sarli, 2010). In contrast to simple empirical or lumped-parameter models, CFD models take into account the interplay between flame propagation and flow field, which is the key process determining dynamics and effects of an explosive phenomenon.

Thanks to the growing power of parallel computers, the CFD approach of Large Eddy Simulation (LES) is becoming a viable method to model turbulent combustion. LES captures the intrinsically unsteady nature of turbulent flows and, thus, is fit for modeling time-dependent combustion phenomena such as oscillations in gas turbine combustors (Selle et al., 2004; Boudier et al., 2007, 2008; Staffelbach et al., 2009), cycle-to-cycle variations in spark-ignition engines (Richard et al., 2007; Goryntsev et al., 2009; Vermorel et al., 2009; Hasse et al., 2010; Enaux et al., 2011) and flame propagation in gas explosions (Masri et al., 2006; Di Sarli et al., 2007b, 2009a, 2009b, 2010; Gubba et al., 2008, 2009; Di Benedetto and Di Sarli, 2010). The attraction of LES is that it offers an improved representation of turbulence, and the resulting flame–turbulence interaction, with respect to classical (and less computationally demanding) Reynolds-averaged Navier–Stokes (RANS) approaches.

LES explicitly resolves the large turbulent structures in a flow field, from the length scale of the computational domain down to a cut-off length scale (i.e., the filter scale) linked to the size of the grid cell, and only models the small sub-grid structures (that, however, exhibit a more universal behavior). The grid resolution represents the scale separation between the length scales of computed (resolved) turbulence and those of modeled (unresolved) turbulence. It is, therefore, a critical parameter in determining the quality of any LES computation that mostly relies on the percentage of the resolved

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0009-2509/$ - see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ces.2011.11.034

turbulent kinetic energy. Resolving at least 80% of the turbulent kinetic energy can be considered as a good LES (Pope, 2004). As the grid size decreases, the percentage of the resolved turbulent kinetic energy increases and the contribution from the sub-grid model reduces, eventually reaching the asymptote of Direct Numerical Simulation (DNS) (i.e., percentage of the resolved turbulent kinetic energy equal to 100% and, thus, no need for sub-grid turbulence models) (Pope, 2004).

When the evolution of a turbulent flow field is coupled to flame propagation, the predictive capability of LES also relies on the combustion sub-model implemented. Indeed, LES does not resolve the flame front on the numerical grid, the premixed flame thickness being smaller than the grid size used. Consequently, the flame and its interaction with the sub-grid vortices have to be modeled (Poinsot and Veynante, 2005; Pitsch, 2006), whereas the effects of the large vortices on the flame propagation are directly computed.

For LES of unsteady premixed flame propagation in gas explosions, we have shown that the role of the combustion sub-model is mainly to affect the results in quantitative terms rather than in qualitative terms (Di Sarli et al., 2009a, 2010). In our model, the combustion rate was kept constant on the value of the laminar burning velocity and a sub-grid flame wrinkling factor was introduced to take into account the effects of the unresolved turbulence on combustion. Even without the combustion sub-model (i.e., even when setting the sub-grid wrinkling factor equal to unity), good agreement between LES predictions and experimental results has been obtained for the shape and the structure of the propagating flame front, as well as for the qualitative trends of both the flame speed profile and the pressure time history (Di Sarli et al., 2009a). This means that, within the range of conditions investigated (in any case far from the onset of detonation), the increase in overall energy release rate is dominated by the growth in flame surface area that is, in turn, determined by the (resolved) flow field and not by the combustion rate itself. However, for the grid resolution employed, we have found that the combustion sub-model is needed and its choice is a crucial point to obtain quantitative predictions that correctly match the experimental data (Di Sarli et al., 2010).

Reducing the grid size can affect the relevance of the combustion sub-model, possibly leading to an asymptotic solution (Richard et al., 2007) (as in LES of non-reactive flows) that is independent of the presence of the combustion sub-model itself.

The effects of grid resolution on LES of gas explosions have been assessed in the works by Masri's group (Masri et al., 2006; Gubba et al., 2009). These papers attempt to shed more light on the issue of obtaining grid-independent solutions. Better agreement between LES predictions and experimental data (time traces for overpressure, flame location and flame speed) has been found with decreasing grid size. However, for grid size approaching the laminar flame thickness, this gain does not seem to justify the added computational cost (Gubba et al., 2009).

In the present work, the opportunity of reaching a solution independent of the presence of the combustion sub-model for LES of transient flame–vortex interactions in gas explosions was investigated. To this end, the LES model of unsteady premixed flame propagation developed and validated in Di Sarli et al. (2009a, 2010) was used. LES computations were run on three grids of increasing resolution up to cell size-to-laminar flame thickness ratio equal to unity. The predictive capability of the LES model was evaluated by comparing numerical results with the experimental data acquired by Long et al. (2006) during the interaction of a propagating flame front with toroidal vortices generated at the wake of a circular orifice. To quantify the role of the combustion sub-model as a function of the grid resolution, large eddy simulations were also run without the combustion sub-model on all three grids.

2. Test case

Numerical results were compared with the experimental data acquired by Long et al. (2006) using the test rig schematized in Fig. 1a. Within this rig, a quiescent premixed charge of stoichiometric methane and air was ignited inside a small cylindrical pre-chamber (35 mm in height and 70 mm in diameter) linked to the main chamber (150 mm × 150 mm × 150 mm) *via* a small orifice (30 mm in height and 30 mm in diameter). The orifice had sharp edges at both the pre-chamber and main chamber sides. The bottom end of the pre-chamber was fully closed. The upper end of the main chamber was sealed by a thin PVC membrane that ruptured soon after ignition, allowing the exhaust gases to escape. The main chamber was constructed from polycarbonate to provide optical access.

The mixture was ignited at the center of the bottom end of the pre-chamber. After ignition, the flame propagated through the pre-chamber, pushing unburned charge ahead of the flame front through the orifice. This motion of the reactants through the constriction resulted in a toroidal vortex being shed into the main chamber. As the flame continued to propagate through the charge, it interacted with the vortex structure (Fig. 1b), distorting the flame and altering its burning velocity.

In order to characterize and quantify the interaction between the flow field and the flame front, two high speed laser diagnostic techniques were employed: High Speed Laser Sheet Flow Visualization (HSLSFV) and High Speed Digital Particle Image Velocimetry (HSDPIV).

The HSLSFV technique provided a global visualization of the flame front development throughout the combustion event. It consisted of an Oxford Lasers Copper Vapor Laser LS20-40 synchronized to a Kodak Ektapro 4540 high speed motion analyzer. The output of the copper vapor laser was introduced through the sidewall of the main chamber in the form of a thin sheet, created using a spherical and then a cylindrical lens. Flow tracer particles

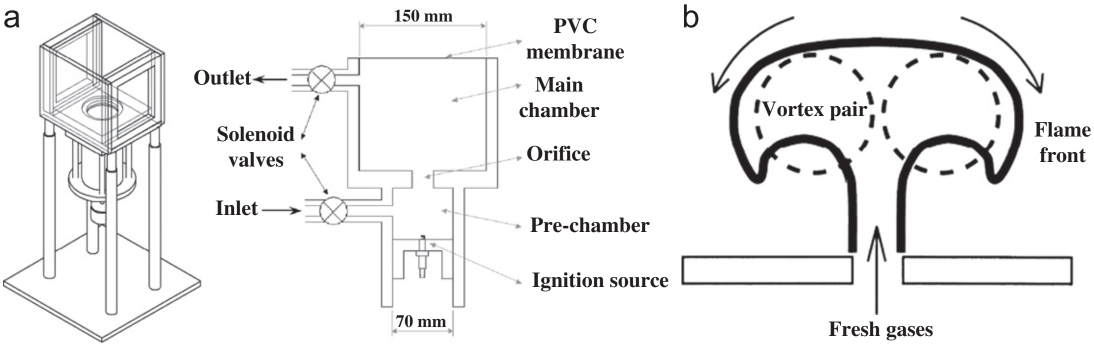

Fig. 1. Schematic representations of the test rig by Long et al. (2006) (not to scale) (a) and of the flame–vortex interaction (b).