Large Eddy Simulation of Gas Explosions

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This paper reviews the most important advancements obtained by means of Safety Computational Fluid Dynamics (Safety CFD, SCFD) models based on the Large Eddy Simulation (LES) approach in the study of gas explosions at both laboratory and industrial scales.

It is pointed out the central role of LES as the most adequate tool for describing the inherently unsteady interplay of flame propagation, flow field and geometry, associated to explosion phenomena. Some issues yet to be addressed are discussed as relevant to fully realize the potential of explosion LES.

1. Introduction

Gas explosions are complex phenomena involving several spatial and time scales as well as strong gradients of field variables (fluid density, velocity, pressure, temperature and species concentration). In addition, they are characterized by the unsteady interaction between the propagating flame and the turbulence induced by the presence of obstacles in the flame path (vessels, pipes, tanks, flow cross-section variations, instrumentations, etc.). The flame-turbulence interaction may lead to significant increase of flame speed and rate of pressure rise. It also modifies the flame structure. For such features, gas explosions are *new* phenomena in the field of turbulent combustion modeling. This justifies the development of *new* tools of Safety Computational Fluid Dynamics (Safety CFD, SCFD) modeling to take into account the dynamic interplay of chemical reaction, transport phenomena, flow field and geometry associated to explosions.

Thanks to the growing computational power and the availability of distributed computing algorithms, advanced SCFD models based on Large Eddy Simulation (LES) are emerging as useful methods for predicting and understating gas explosions.

LES offers an improved representation of turbulence, and the resulting flame-turbulence interaction, with respect to classical Reynolds-Averaged Navier-Stokes (RANS) approaches. Furthermore, LES captures the inherently unsteady nature of turbulent flows and, hence, of transient combustion phenomena such as explosions.

In the following, we review the most important advancements obtained by means of SCFD models based on LES in both the research area and the applicative area. We also discuss some relevant issues yet to be addressed as relevant to fully realize the potential of explosion LES.

2. Advancements in Modeling Laboratory Scale Explosions

SCFD for research should have as main goal to gain insight into the different mechanisms and phenomena coming into play during explosions.

SCFD models allow correlating the spatio-temporal evolution of the flame to its speed and the pressure time history. In addition, they allow the artificial suppression of one mechanism/phenomenon at a time, thus drawing conclusions about the relevance of the mechanisms and phenomena involved (Di Benedetto et al., 2005; Ferrara et al., 2006; Di Sarli et al., 2009a; 2009b).

In the literature, the SCFD models developed for laboratory scale gas explosions are based on both unsteady RANS (URANS) (see, e.g., Popat et al., 1996; Pritchard et al., 1996; Fairweather et al., 1999; Naamansen et al., 2002; Patel et al., 2002; Di Benedetto et al., 2005; Ferrara et al., 2006) and LES (Kirkpatrick et al., 2003; Masri et al., 2006; Gubba et al., 2008; Di Sarli et al., 2009a; 2009b; Ibrahim et al., 2009) approaches.

LES overcomes the difficulties of URANS in capturing features of the flame propagation (steps of acceleration-deceleration around the obstacles, asymmetric shape of the flame, wrinkling of the front, pocket formation) relevant to correctly predict the flame speed and the pressure peak without any *ad hoc* tuning of model constants and parameters (Patel et al., 2002; Di Sarli et al., 2009a).

The LES technique explicitly resolves the large turbulent structures in a flow field (up to the grid dimension), modeling the small structures that, however, exhibit a more universal behavior (Pope, 2000). Unfortunately, chemical reactions in combustion processes occur at characteristic scales that are generally smaller than the affordable mesh resolution. Thus, as in URANS, the LES flame remains a sub-grid phenomenon whose coupling with the unresolved turbulence has to be exclusively modeled (Poinsot and Veynante, 2005). The choice of the sub-grid combustion model is the crucial point for LES of gas explosions.

In all the LES-based SCFD models proposed for simulating laboratory scale explosions (Kirkpatrick et al., 2003; Masri et al., 2006; Gubba et al., 2008; Di Sarli et al., 2009a; 2009b; Ibrahim et al., 2009), the flame surface density formalism based on the *flamelet* concept was chosen and coupled to sub-grid combustion models developed for steady (or quasi-steady) turbulent combustion applications (combustors, burners).

In most of these works (Kirkpatrick et al., 2003; Masri et al., 2006; Gubba et al., 2008), the algebraic closure for the sub-grid flame surface density by Boger et al. (1998) was adopted. Although this sub-grid combustion model exhibits a weak dependence of the combustion rate on the unresolved vortices, the results obtained show satisfactory predictions in terms of flame position, structure and interactions with flow and turbulence. The discrepancies found with regard to the pressure trend have been attributed to the sub-grid combustion model implemented. Ibrahim et al. (2009) have obtained more accurate predictions using the dynamic flame surface density formulation by Knikker et al. (2004).

In our LES study of unsteady flame propagation around obstacles (Di Sarli et al., 2009a; 2009b), the sub-grid wrinkling factor was treated according to the power-law flame wrinkling model by Charlette et al. (2002). Numerical and experimental results agree well in terms of shape of the propagating flame, flame arrival times, spatial profile of the flame speed, pressure time history, and velocity vector fields ahead of the flame front (Di Sarli et al., 2009a).

We also ran large eddy simulations with the sub-grid combustion model eliminated (i.e., by assuming the sub-grid wrinkling factor as constant and equal to unity during the entire propagation) (Di Sarli et al., 2009a). The results obtained demonstrate that the large scale vortices play the dominant role in dictating all trends, including the evolution of the flame structure along the path. Conversely, the sub-grid vortices do not affect the qualitative trends. However, it is essential to model their effects on the combustion rate to achieve quantitative predictions for both flame speed and pressure peak.

The methodology of implementing sub-grid combustion models developed for steady turbulent flames in SCFD codes seems to be successful, even if it has yet to be tested under various conditions and, mainly, at different geometry scales.

The question of the optimal sub-grid combustion model for explosion LES still remains open. Research effort is required to develop, test and compare sub-grid combustion models according to the criteria of level of description, completeness, cost and ease of use, range of applicability, and accuracy (Pope, 2000).

3. Advancements in Modeling Large Scale Explosions

For industrial scale explosions, modeling becomes much more important, since large scale experiments are costly and often unpractical.

When scaling from laboratory up to industrial scales, two main issues arise.

The first issue is related to the need of modeling phenomena which are negligible at laboratory scales and become important at large scales. In large scale enclosures, the flammable gas scarcely becomes uniform (Hirano, 2008). Furthermore, the flame interaction with pressure waves, which increases the flame front wrinkling and corrugation and, thus, the burning velocity, is much stronger at large than at small scales (Kumar et al., 1989; Teerling et al., 2005).

The second issue arising in the scale-up is the computational cost. LES needs fine grids, given that the small turbulent structures become independent of the flow and geometry starting from a size equal to around ≈ 10 mm (Pope, 2000). This issue strongly limits the application of LES to large scale explosions.

Most of the SCFD models developed for large scale phenomena are based on the URANS approach (see., e.g., Bakke and Hjertager 1986; Hjertager, 1989; 1991; Hjertager et al., 1992; Catlin et al., 1995; Popat et al., 1996; Salzano et al., 2002). Only recently, the LES approach has been proposed for large scale explosions (Makarov and Molkov, 2004; Molkov and Makarov, 2006). In these works, the effects of mixture non-uniformity and flame front-pressure wave interaction were not taken into account. Furthermore, rather coarse grids were employed as a result of a trade-off between the need to apply LES at large scales and the available computational power.

In Makarov and Molkov (2004), an LES model of gaseous deflagration in a closed spherical vessel ($V \approx 6.5\ \mathrm{m}^3$) was developed with the sub-grid wrinkling factor assumed as constant and equal to unity. The grid was adapted to the local gradient of reaction progress variable, providing a finer resolution (average linear size of the adapted grid cell $\approx$ 35 mm) in the area around the flame front with moderate CPU time. The model reproduces the experimental pressure dynamics with an error smaller than 10 %. In addition, it explicitly resolves the cellular structure of the spherical flame front.

Molkov and Makarov (2006) ran LES computations of vented gas explosions in the SOLVEX enclosure ($V \approx 550\ \mathrm{m}^3$). In these *very large* eddy simulations, a grid cell dimension of around 0.7 - 0.8 m was chosen. The sub-grid wrinkling factor was assumed as a function of the local turbulent conditions according to the model by Yakhot (1988). The LES model is unable to correctly predict the pressure peak without the introduction of an additional wrinkling factor outside the enclosure, where more intense vortical structures arise.

4. Conclusions

In the field of small scale explosions, LES has shown its superiority with respect to URANS. LES can be seen as a truly predictive tool. On the contrary, URANS is simply an *a posteriori* descriptive tool: in order to reproduce flame speeds and pressure peaks, it needs experimental data against which to compare and validate numerical results by an *ad hoc* tuning of model constants/parameters. Therefore, results cannot be extrapolated outside their range of validation.

Thanks to the continuous growth of computational power and the development of ever more robust distributed computing algorithms, it can be expected to extend LES to large scale explosions in the near future. This poses a number of challenges for modelers (for example, non-uniformity of the flammable gas, interaction between flame front and pressure waves).

In the meantime, since URANS still remains the only feasible methodology for modeling real scale explosions, it should be used with the full awareness of its limitations.

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