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Large eddy simulation of explosion deflagrating flames using a dynamic wrinkling formulation

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ABSTRACT

Reliable predictions of flames propagating in a semi-confined environment are vital for safety reasons, once they are representative of accidental explosion configurations. Large eddy simulations of deflagrating flames are carried out using a dynamic flame wrinkling factor model. This model, validated from a posteriori analysis, is able to capture both laminar and turbulent flame regimes. At early stages of the flame development, a laminar flame propagates in a flow essentially at rest and the model parameter is close to zero, corresponding to a unity-wrinkling factor. Transition to turbulence occurs when the flame interacts with the flow motions generated by thermal expansion and obstacles. The model parameter and wrinkling factor take higher values at these stages. Three configurations investigated experimentally by Masri et al. 2012, corresponding to different scenarios of flame acceleration are simulated. The first case (OOBS) is characterized by a long laminar phase. In the second one (BBBS) the flame is the most turbulent and the highest overpressure is observed in the vessel. For the last case (BOOS), the flame front is relaminarized after crossing the first row of obstacles. In all configurations, large eddy simulations (LES) predict the flow dynamics and maximum overpressure with good accuracy.

1. Introduction

Accidental explosions of flammable gases are a current issue in process industries. Selecting the optimal conditions and parameters in the design and operation of chemical, petrochemical, mining, nuclear and others industrial plants is not only a matter of safety but also economical and environmental issues. In gas explosions of a premixed gas cloud, the pressure increase is governed by a complex unsteady interaction between flame propagation, turbulence and geometry. This overpressure is often considered as the key parameter, since it controls the severity of the explosion and corresponding damages. This complex phenomenon is very challenging for computational fluid dynamics (CFD) problems since it involves a large spectrum of spatial and time scales and encompasses a large range of flow and combustion regimes.

The typical research configuration used to study explosions in buildings consist in vessels with obstacles filled with a premixed flammable mixture. After the ignition, a laminar flame propagates in a flow essentially at rest. Transition to turbulence takes place when the flame starts to interact with obstacles and their wakes. This interaction strongly influences the shape of the flame front, the burning rate and, as a consequence, the overpressure. This flame induced flow field increases turbulence and combustion intensity, leading to flames, which can propagate at 100–200 m/s. In the worst scenario, the initial flame can transition to detonation and cause the destruction of the whole building.

A large number of experiments have been carried out in order to understand flame/turbulence interactions in vented explosion chambers with solid obstacles [1–8]. Effects of geometry [1–4] and fuel type [2–4] have been analyzed in order to point out mechanisms involved in the overpressure generation. Flame acceleration and deflagration to detonation transition are also subjects of several reviews [6–8]. This work focuses on the configurations studied experimentally by Masri and co-workers [2,4]. Different geometries, fuel types and scales were reported. The experiments have access to the pressure evolution inside the chamber, the flame speed and flame front position along the middle section of the chamber. Additionally, they have well prescribed initial and boundary conditions and for this reason are very appropriate for model validation.

On the numerical side, thanks to the growing computational power and the availability of parallel computing algorithms, large eddy simulation (LES) is becoming a routinely used tool to predict

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and reproduce turbulent reactive flows [9–12]. In LES, the large turbulent structures of the flow are resolved and the effect of small structures that exhibit a more universal behavior are modeled. Unfortunately, chemical reactions in combustion processes occur at characteristic scales that are smaller than the mesh resolution and a good combustion model is vital to capture the physics of the flow. Several numerical studies dealing with deflagrations in semi-confined chambers are reported in the literature [13–25].

The majority of LES of premixed flame deflagration in the presence of obstacles relies on the Flame Surface Density (FSD) approach. In this case, the species transport equations are simplified in the form of a transport equation for the reaction progress variable, which is zero within fresh reactants and unity within burned products [13–24]. The only exception is Quillatre et al. [25] that use the Thickening Flame model for LES (TFLES) together with reduced kinetic schemes for CH_4 - C_3H_8 and H_2/air combustion. While the former method has the advantage of being computationally cheaper, the latter one takes into account molecular and thermal transports, which turn out to have a significant impact on the results [25].

Di Sarli et al. [16] highlighted the importance of the sub-grid closure in the reproduction of the experiment studied by Patel et al. [26], in terms of flame acceleration and deceleration around each obstacle, flame shape and speed as well as pressure peak. Actually, most of the models employed in their study needed parameter adjustments to obtain more realistic trends. Di Sarli et al. [21–23] also carefully validated LES FSD algebraic models of explosion deflagrating flames against precise time- and space-resolved experimental data including images of the propagating flame front and velocity vector maps. They note that, when the grid resolution is of the order of the laminar flame thickness, numerical results correctly match experiments even without sub-grid scale combustion model [21] but the generation of turbulence induced by the thermal expansion is mainly limited to a large scale vortex in their configuration.

As a matter of fact, LES models based on algebraic expressions for the turbulent flame speed [27,28], the flame surface density [29] or the flame surface wrinkling factor [30,31] are derived assuming local equilibrium between flame surface and turbulence motions. Model expressions depend on local turbulence characteristics such as turbulence intensity and length scales evaluated during simulations. Reaction rates then vary with space and time but may be erroneous when equilibrium is not reached, requiring the adjustment of model parameters for any small change in the operating conditions or in the geometry [32]. Models based on a balance equation for the flame surface density [33–35] or the wrinkling factor measuring the ratio of total and resolved flame surfaces [36], release this equilibrium assumption by construction but require additional closures. In practice, some model coefficients may still have to be adjusted when operating conditions change. For example, Mouriaux et al. [37] adjusted one parameter in the flame surface density transport equation when varying internal combustion engine speed.

Dynamic models, which take advantage of the known resolved large scales to automatically adjust model parameters, are an attractive alternative for these situations. The model is written at LES and test-filtered scales and the parameter is the solution of a Germano-like equation [38]. Validated in simple flow configurations (flame embedded in a homogeneous isotropic turbulence) [39–41], dynamic models have proven to be very effective in reproducing steady stable [42–46] and unstable [47] flames. They were successfully employed to simulate transient phenomena as well. Mouriaux et al. [37] obtained very good results, when dealing with internal combustion engines at distinct speeds. Gubba et al. [19], Ibrahim et al. [20] obtained accurate predictions using the dynamic FSD similarity formulation developed by Knikker et al. [48] for various explosion configurations studied experimentally by Masri et al. [4].

This work aims to validate the local dynamic wrinkling factor approach coupled with the Thickened Flame (TFLES) combustion model in the explosion test-cases studied experimentally by Masri et al. [4]. This combination has already been employed in other studies [39,43,46,47]. The present manuscript is organized as follows: basic concepts of TFLES and the dynamic approach are discussed in Section 2. In Section 3, the experimental test cases are presented. Then, the chemical scheme employed in our computations is presented (Section 4). In Section 5, a sensitivity analysis, regarding mesh sizes, transport models, boundary conditions and other features of numerical simulations, is carried out on 2D-DNS and 2D-LES configurations and serves as basis for the three-dimensional study. The numerical set-up for the three-dimensional configurations is introduced in Section 6. Finally, a posteriori results for different geometries, corresponding to three scenarios of flame acceleration, are discussed (Section 7). Conclusions are drawn.

2. Modeling

2.1. The thickened flame model (TFLES)

One of the challenges in large eddy simulations of premixed combusting flows is the fact that the flame front cannot be resolved on the computational mesh. A common procedure to overcome this problem is to artificially thicken the flame by multiplying diffusion and dividing reaction rates by a thickening factor $\mathcal{F}$ [49]. The modified flame front of thickness $\mathcal{F}\delta_L^0$ propagates at the same laminar flame speed S_L as the original flame of thickness δ_L^0. However, the Damköhler number is modified and the flame becomes less sensitive to turbulence [30]. A wrinkling factor Ξ_Δ is then introduced to counterbalance the reduction of flame surface induced by the thickening operation [30,31]. The balance equations for filtered species mass fractions $\widetilde{Y}_k$ are written as:

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \nabla\cdot(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Y}_k) = -\nabla\cdot(\Xi_\Delta\mathcal{F}\overline{\rho\mathbf{V}_k\widetilde{Y}_k}) + \frac{\Xi_\Delta}{\mathcal{F}}\dot{\omega}_k(\widetilde{Q}) \tag{1}$$

where ρ is the density, $\mathbf{u}$ the velocity vector, $\mathbf{V_k}$ the diffusion velocity of species k, expressed here using the Hirschfelder and Curtiss approximation [11] and $\dot{\omega}_k$ the reaction rate of species k. Any quantity $\overline{Q}$ corresponds to the filtered Q-field, while $\widetilde{Q} = \overline{\rho Q}/\overline{\rho}$ denotes mass-weighted filtering. Eq. (1) propagates a flame front of thickness $\mathcal{F}\delta_L^0$ at the sub-grid scale turbulent velocity $S_T = \Xi_\Delta S_L$. The balance equation for the filtered total energy is modified in the same manner.

2.2. Dynamic wrinkling model

The wrinkling factor Ξ_Δ models the ability of sub-grid scale vortices to wrinkle the flame front. This term is usually modeled in the literature by complex algebraic expressions. Generally, these expressions involve other unresolved terms (for instance, the sub-grid scale turbulent velocity, u'_Δ), which also need modeling. The sub-grid scale wrinkling factor Ξ_Δ is modeled as:

$$\Xi_\Delta = \left(\frac{\Delta}{\delta_c}\right)^\beta \tag{2}$$

where β is the model parameter. In the present work, the inner cut-off δ_c (i.e. the smallest scale for the interaction of turbulent eddies with the premixed flame front) is identified to the laminar flame thickness, an assumption validated using two-dimensional simulations (see Section 5.6) and in agreement with other studies [39,50]. When β is independent on the scale Δ and verifies $0 \leq \beta \leq 1$, Eq. (2) recover the fractal model [51–53], where