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Numerical simulation of premixed methane–air deflagration in a semi-confined obstructed chamber

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ABSTRACT

In this paper, large eddy simulation coupled with a turbulent flame speed cloure (TFC) subgrid combustion model has been utilized to simulate premixed methane–air deflagration in a semi-confined chamber with three obstacles mounted inside.

The computational results are in good agreement with published experimental data, including flame structures, pressure time history and flame speed. The attention is focused on the flame flow field interaction, pressure dynamics, as well as the mechanism of obstacle-induced deflagration. It is found that there is a positive feedback mechanism established between the flame propagation and the flow field. The pressure time history can be divided into four stages and the pseudo-combustion concept is proposed to explain the pressure oscillation phenomenon. The obstacle-induction mechanism includes direct effect and indirect effect, but do not always occur at the same time.

1. Introduction

Methane–air deflagration accidents frequently occur in coal mines and natural gas pipelines and cause considerable losses of life and property. In these accidents, the interaction of deflagrating flame and obstacles resulted in significant changes in the structure of flame, pressure rise and flame propagation speed, contributing to more serious damage. Therefore, the comprehension of the obstacle-induced mechanism is essential for industrial safety.

In the past decades, a great number of studies, both experimental and numerical, have been carried out dealing with flame–obstacle interactions. Experiments have been performed in various conditions and geometrical configurations. Recently, Hall et al. (2009) studied the influence of the number and location of obstacles on the rate of flame propagation in a vented chamber. They found that the peak pressure will reach a limit with increasing number of obstacles and the location of obstacles has an impact on the overpressure and flame structure, as extending the distance between obstacles allows turbulence relaminarization. Johansen, and Ciccarelli (2009) performed experiments in a closed obstructed square cross-section duct with different blockage ratios. The influence of the blockage ratio on the early period of flame acceleration was analyzed and it was found that recirculation zones of flow field ahead the flame front has an important effect on the combustion with enhanced turbulence and enlarged flame areas. Wen et al. (2013) investigated the effects of obstacle positions on methane–air deflagration in a semi-confined channel with three obstacles. It is found that the greatest peak pressure occurs in the configuration with staggered obstacles and highest flame propagation speed in the configuration with centrally located obstacles. In a recent study, the obstacle separation is also demonstrated to be an important factor (Na'inna et al., 2013). It shows that there is a defined separation distance which will result in more severe explosion effect in terms of highest flame speed and maximum pressure.

On the numerical side, URANS approaches have been employed in many past works (Fairweather et al., 1999; Patel et al., 2002) and recently, because of the need for more accurate prediction, Large-eddy simulation (LES) attracts a significant interest and has been applied to a variety of combustion problems (Pitsch, 2006). Di Sarli et al. (2009a) modeled deflagration in a small scale vented chamber with single obstacle, the effects of methane–air mixtures with different equivalence ratios, different obstacle blockage ratios and

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different obstacle shape are investigated. The authors originally related the overpressure changes to the competition between combustion rate and venting rate. For applications of LES in combustion simulation, one of the most important steps is the reaction rate quantification which requires a subgrid scale combustion model (Poinsot and Veynante, 2005). Five different subgrid scale (sgs) combustion models proposed for LES were performed to identify the best model that predicts unsteady flame propagation through obstacles (Di Sarli et al., 2010). Wen et al. (2012) simulated the methane–air deflagration in a vented chamber with three obstacles using LES with three sub-grid scale combustion models and interaction between flame propagation and turbulence induced by obstacles was studied. Johansen and Ciccarelli (2013) calculated the initial flame acceleration in a confined channel using LES coupled with dynamic Smagorinsky-Lilly subgrid model and the Boger flame surface density combustion model. This paper focus on the influence of unburned gas flow field development on the flame construction and initial acceleration under various obstacle blockage ratio conditions.

In the present work, large eddy simulation of methane–air deflagration in a semi-confined chamber with three obstacles is carried out with a turbulent flame speed cloure (TFC) subgrid combustion model proposed by Zimont and Battaglia (2006). The numerical results are compared to experimental data aiming to validate the model. In addition, the details of flame shape, pressure rise and flame acceleration are analyzed and the mechanism of obstacle-induced deflagration will be discussed.

2. Experimental case

Simulations are run of the experiment with stoichiometric methane–air deflagration in a vented chamber conducted by Patel et al. (2002). A schematic diagram of the chamber is shown in Fig. 1. The chamber was 150 mm × 150 mm in cross-section and 500 mm in height. Three rectangular obstacles (150 mm × 75 mm × 10 mm) were positioned at 100 mm regular spacing in the chamber and the blockage area ratio was 0.5. The bottom end of the chamber was fully closed and the upper end was sealed by a thin PVC membrane which ruptured during the deflagration process allowing the gases to escape. A stoichiometric methane–air mixture was purged through the chamber and ignited at the center of the bottom end. A high-speed laser-sheet flow visualization system was utilized to capture the flame propagation images at an image recording rate of 9000 Hz and pressure time history was obtained by using a high-speed piezoelectric pressure transducer located close to the ignition point.

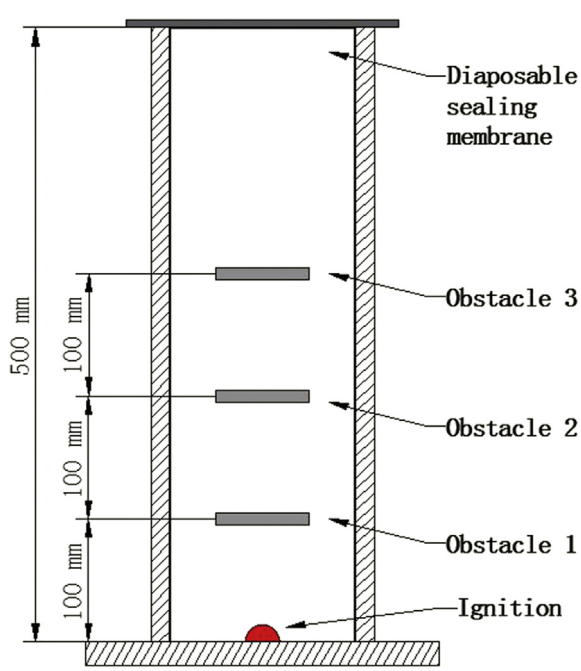

Fig. 1. Schematic diagram of the chamber.

3. Large eddy simulation (LES) and combustion model

The LES model used in this work has been described previously (Bi et al., 2012; Di Sarli et al., 2009a). The model equations are obtained by applying a Favre-filter (i.e. mass-weighted filtered) to the conservation equations of mass, momentum, energy and species, joined to the constitutive and state equations. The flame propagation is modeled by the recast species transport equation in the form of a transport equation for the reaction progress variable, c, which is defined as a normalized mass fraction of products such that c equals zero in the fresh reactants and one in the burned products:

$$c = \frac{\sum_{i=1}^{n} Y_i}{\sum_{i=1}^{n} Y_{i,eq}} \tag{1}$$

where n is the number of products; Y_i is the mass fraction of product specie i, $Y_{i,eq}$ is the equilibrium mass product specie i. The LES Favre-filtered conservation equation for c reads:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{c}) = \frac{\partial}{\partial x_j}\left(-\frac{\mu+\mu_t}{Sc_t}\frac{\partial\tilde{c}}{\partial x_j}\right) + \bar{S}_c \tag{2}$$

where ρ is the density, u is the velocity, μ is the molecular viscosity, μ_t is the turbulent viscosity, Sc_t is the turbulent Schmidt number and S_c is the reaction progress variable source term. The overbar (−) denotes a LES filtered quantity and the tilde (~) denotes a Favre-filtered quantity. The turbulent viscosity μ_t is modeled applying dynamic Smagorinsky-Lilly model (Lilly, 1992). The turbulent Schmidt number Sc_t is obtained by applying the dynamic procedure originally proposed by Germano et al. (1991). The reaction progress variable source term is modeled as:

$$\bar{S}_c = \bar{\rho}_u U_t |\nabla\bar{c}| \tag{3}$$

where ρ_u is the density of unburned mixture, U_t is the turbulent flame speed obtained by a TFC model proposed by Zimont and Battaglia (2006):

$$U_t = A(u')^{3/4} U_l^{1/2} \alpha^{-1/4} l_t^{1/4} \tag{4}$$

where A is an empirical parameter and equals 0.5, which is recommended by Zimont (2000) for hydrocarbon fuels (CH4,C2H6,C3H8); u' is the subgrid velocity fluctuation; U_l is the laminar flame speed and equals 0.41 m/s for stoichiometric methane–air mixture (Yu et al., 1986); α is the thermal diffusivity of unburnt mixture; l_t is the turbulence length scale modeled as:

$$l_t = Cs\Delta \tag{5}$$

where Cs is the Smagorinsky constant dynamically computed based on the information provided by the resolved scales of motion (Lilly, 1992), and Δ is the cell characteristic length.

The subgrid velocity fluctuation is calculated as: