Process Safety and Environmental Protection 120 (2018) 45–56

Contents lists available at ScienceDirect

Process Safety and Environmental Protection

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

Comparative study of the propagation of methane/air and hydrogen/air flames in a duct using large eddy simulation

Kai Zheng[a], Minggao Yu[a,b,*], Ligang Zheng[b], Xiaoping Wen[c]

[a] *State Key Laboratory of coal mine disaster dynamics and control, Chongqing University, Chongqing 400044, PR China*
[b] *School of Safety Science and Engineering, Henan Polytechnic University, Jiaozuo 454003, PR China*
[c] *School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo 454003, PR China*

ARTICLE INFO

Article history:
Received 4 June 2018
Received in revised form 16 August 2018
Accepted 22 August 2018
Available online 3 September 2018

Keywords:
Methane/air
Hydrogen/air
Large eddy simulation
Flame propagation

ABSTRACT

The propagation of methane/air and hydrogen/air explosion flames in four closed ducts with different aspect ratios was numerically investigated using large eddy simulation (LES). The numerical model was validated by comparing the numerical results with the experimental results, and reasonable agreement is observed between them. For methane/air, only the tulip shaped flame (concave flame front) can be observed after the flame inverts and no oscillation occurs. The tulip lips distortion occurs in the duct with aspect ratio (the ratio of length to width) of 7.5 in hydrogen/air, and the deformation becomes more distinguished as the aspect ratio increases. Consistent with the flame structure evolution, the flame speed and rate of pressure rise decrease after the flame touches the sidewalls in methane/air. For hydrogen/air, with the emergence of tulip lips distortion, an oscillation appears in the flame propagation speed and pressure curves when the aspect ratio is 7.5. Moreover, the oscillation becomes stronger as the aspect ratio increases. With this increase in the aspect ratio, the interaction between flame and pressure wave leads to the emergence of different flow patterns after the tulip shaped flame formation.

1. Introduction

With the development of the economy, the problems of environmental pollution, climate anomalies and energy shortages have become increasingly serious, making the exploitation of renewable clean energy important. Currently, as the main component of natural gas, methane is recognized as a type of clean fuel source and is widely applied in industry. In addition, as a promising clean fuel, hydrogen has a higher heating value per kilogram and produces fewer pollutants; as a result, it has attracted the attention of many scholars, and investigating its combustion characteristics has become a research topic (Alipoor and Saidi, 2017; Dayma et al., 2014; Frouzakis et al., 2015). However, the safe application of a fuel is mainly dependent on its explosion characteristics. In industrial applications, most explosion accidents are associated with massive rapid releases of energy of a flammable mixtures that begins as a deflagration (Ng and Lee, 2008). Under certain conditions, the explosion could accelerate and transition from deflagration to detonation (Ciccarelli and Dorofeev, 2008), which is the most destructive manner of a gas explosion. Hence, from the viewpoint of safety, it is of great importance to investigate the explosion behaviors of methane/air and hydrogen/air.

Over the past decades, extensive research studies have been performed to characterize the flame propagation during gas explosions (Alharbi et al., 2014; Blanchard et al., 2010; Boeck et al., 2014; Carcassi and Fineschi, 2005; Kim et al., 2013; Kuznetsov et al., 2015; Yu et al., 2017). A flame can display various shapes when propagating in a closed duct after ignition, e.g., in the form of a hemisphere, finger, or “tulip” (Clanet and Searby, 1996). After ignition, the flame propagates with a hemispherical shape. Subsequently, the flame develops into a finger shape and accelerates exponentially (Bychkov et al., 2007). The acceleration process stops as the flame touches the duct sidewalls, which is followed by flame front inversion and eventually results in the formation of the classic “tulip” flame. Previous studies on the “tulip” flame are based largely on methane/air and propane/air mixtures (Gonzalez et al., 1992; Markstein, 1957; Ponizy et al., 2014; Starke and Roth, 1986). For hydrogen/air explosion flame propagation in a closed duct, flame distortion occurs after a “tulip” flame is well established. Xiao et al. (2011) named this structure the “distorted tulip” flame. At the onset of the “distorted tulip” flame formation, oscillations appear in both flame and pressure dynamics. The hydrogen/air explosion flame propagation in closed ducts is simulated by solving the fully

---

* Corresponding author at: 174 Shazhengjie, Shapingba, Chongqing, 400030, PR China.
E-mail address: 13333910808@126.com (M. Yu).

https://doi.org/10.1016/j.psep.2018.08.025

compressible reactive Navier-Stokes equations; it is found that the tulip lips distortion can be attributed to the interaction between the flame front and the pressure wave (Xiao et al., 2013, 2015, 2017). Recently, the propagation characteristics of methane/air and hydrogen/air flames were compared based on experimental data (Li et al., 2015; Zheng et al., 2017); the results were found to be largely different between hydrogen/air and methane/air mixtures because of the completely different combustion properties. However, among the studies, because of the limited experimental data, the exact mechanism of the appearance of different flame structures in methane/air and hydrogen/air explosions is still not clear.

With the rapid development of computers and parallel computing, progress has been made in large eddy simulation (LES) of the flame propagation in ducts. Compared to the experimental method, LES can provide more parameters that help to understand the mechanism of flame propagation, e.g., flame structure, pressure dynamics and flow field in the vicinity of the flame. In LES, various modeling approaches, e.g., flame surface density (FSD), thickened flame (TF) and turbulent flame closure (TFC), have been adopted to simulate unsteady flame propagation in gas explosions (Chen et al., 2016; Bi et al., 2012; Li et al., 2017, 2018; Molkov et al., 2006, 2007; Sarli et al., 2012; Tolias et al., 2018; Volpiani et al., 2017; Wen et al., 2012; Xiao et al., 2012). Molkov et al. (2006, 2007) develop a new modeling approach to predict the propagationprocess of a premixed hydrogen/air explosion vented through a duct. Di Sarli et al. (2012) studied the phenomenology underlying the explosions that occur in a small-scale vented chamber using a validated LES model. Bi et al. (2012) performed a LES of gaseous deflagrations in ducts with a large aspect ratio using the turbulent flame closure combustion model. Wen et al. (2012) carried out a LES of methane/air flame propagation in a semi-confined chamber with three solid obstacles. Xiao et al. (2012) experimentally and numerically investigated the dynamics of the hydrogen/air flame in a closed duct using a multi-phenomenon combustion model. Li et al. (2017) investigated the explosion flame propagation of a gasoline-air mixture in an obstructed semi-confined duct by conducting a LES simulation coupled with a TFC sub-grid combustion model. Volpiani et al. (2017) performed LES of turbulent flames propagating past repeated obstacles and validated the local dynamic wrinkling factor approach coupled with the thickened flame model. The above simulation results demonstrate that those models can reproduce the flame features, flame speed and pressure and are useful to explain the dynamics of flame propagation in combustible gas explosions.

In this work, LES were conducted to investigate the influence of the aspect ratio on the propagation of methane/air and hydrogen/air flames in closed ducts. In LES, a power-law flame wrinkling model proposed by Charlette et al. (2002a,b) was employed to capture the dynamics of the flame propagation, and four closed ducts with different aspect ratios were considered, to compare the flame structures of methane/air and hydrogen/air mixtures. The model was validated by comparing the numerical results with experimental results.

2. Numerical model

2.1. Large Eddy simulation (LES) model

Numerical simulations including hydrodynamic and species transport processes were performed for the flame propagation in three-dimensional (3D) ducts. The LES based on a low-pass filtering procedure was applied to model the turbulence. In LES, a filtering operation is performed on the Navier-Stokes equations by the LES filter so that the large structures of the flow field can be solved directly, whereas the small ones need to be modeled. The turbulent flame was modeled by introducing a reaction progress variable, c, into the species transport equation, which was zero in fresh fuel/mixtures and unity for combustion products (Sarli et al., 2012). The modeled progress variable equation can be written as (Wen et al., 2012)

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c})+\nabla\cdot(\bar{\rho}\tilde{u}\tilde{c})=\nabla\cdot\left(\frac{\mu_{\mathrm{eff}}}{Sc_{\mathrm{eff}}}\nabla\tilde{c}\right)+\bar{S}_C \tag{1}$$

Here, the overbar (–) denotes a filtered quantity, and the tilde (~) denotes a Favre-filtered quantity. ρ is the mass density, and u is the velocity. μ_{eff} is the effective viscosity, which is derived from the renormalization group theory (Yakhot and Orszag, 1986a) and is given by $\mu_{\mathrm{eff}}=\mu\left[1+H\left(\mu_s^2\mu_{\mathrm{eff}}/\mu^3-100\right)\right]^{1/3}$, where $H(x)$ is the Heaviside function (Sarli et al., 2012), V_{CV} is the volume of the computational cell and μ is the molecular viscosity $\mu_s=\bar{\rho}\left(0.157V_{cv}^{1/3}\right)^2\sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$. $\tilde{S}_{ij}$ is the strain rate tensor, given by $\tilde{S}_{ij}=1/2\left[\left(\partial\tilde{u}_i/\partial x_j\right)+\left(\partial\tilde{u}_j/\partial x_i\right)\right]$. Sc_{eff} is the effective Schmidt number, which is assumed to equal the effective Prandtl number, $P\mathrm{r}_{\mathrm{eff}}$, and is taken as 0.7 (Yakhot and Orszag, 1986b).

The reaction progress variable source term, $\bar{S}_C$, is described by the flame surface density model:

$$\bar{S}_C=\bar{\rho}_{\mathrm{u}}S_l\Xi_\Delta\left|\nabla\tilde{c}\right| \tag{2}$$

where $\bar{\rho}_{\mathrm{u}}$ is the reactant's density and S_l is the laminar flame speed. Ξ_Δ is the sub-grid scale (sgs) wrinkling factor, which is calculated by a power-law flame wrinkling model proposed by Charlette et al. (2002a,b):

$$\Xi_\Delta=\left(1+\min\left[\frac{\Delta}{\delta_f},\Gamma\left(\frac{\Delta}{\delta_f},\frac{u'_\Delta}{S_l},Re_\Delta\right)\frac{u'_\Delta}{S_l}\right]\right)^\beta \tag{3}$$

where $\Delta=(\Delta x\Delta y\Delta z)^{1/3}$ is the filter size. $Re_\Delta=u'_\Delta\Delta/\nu$. is the SGS Reynolds number, and δ_f is the laminar flame thickness that is estimated from $\delta_f S_l/\nu=4$. u'_Δ is the sgs turbulent velocity, which is determined by the Smagorinsky-Lilly eddy viscosity model (Versteeg and Malalasekera, 2007). $\beta$is the model parameter and is set to 0.5, as recommended by Charlette et al. (2002a,b).

The efficiency function, Γ, which describes the net straining effect of all relevant turbulent scales smaller thanΔ, is defined as follows (Charlette et al., 2002a,b):

$$\Gamma\left(\frac{\Delta}{\delta_f},\frac{u'_\Delta}{S_l},\mathrm{Re}_\Delta\right)=\left[\left(\left(f_{\mathrm{u}}^{-\mathrm{a}}+f_\Delta^{-\mathrm{a}}\right)^{-1/\mathrm{a}}\right)^{-\mathrm{b}}+f_{\mathrm{Re}}^{-\mathrm{b}}\right]^{-1/\mathrm{b}} \tag{4}$$

where

$$f_{\mathrm{u}}=4\left(\frac{27C_{\mathrm{k}}}{110}\right)^{1/2}\left(\frac{18C_{\mathrm{k}}}{55}\right)\left(\frac{u'_\Delta}{S_l}\right)^2 \tag{5}$$

$$f^\Delta=\left[\frac{27C_{\mathrm{k}}\pi^{4/3}}{110}\times\left(\left(\frac{\Delta}{\delta_f}\right)^{4/3}-1\right)\right]^{1/2} \tag{6}$$

$$f_{\mathrm{Re}}=\left[\frac{9}{55}\exp\left(-\frac{3}{2}C_{\mathrm{k}}\pi^{4/3}Re_\Delta^{-1}\right)\right]^{1/2}\times Re_\Delta^{1/2} \tag{7}$$

In those expressions, $C_{\mathrm{k}}\approx1.5$ is the Kolmogorov constant. The exponents a and b are obtained from formulas (8) and (9) with

$$\mathrm{a}=0.6+0.2\exp\left(-0.1\frac{u'_\Delta}{S_l}\right)-0.2\exp\left(-0.01\frac{\Delta}{\delta_f}\right) \tag{8}$$

$$\mathrm{b}=1.4 \tag{9}$$

2.2. Numerical details

In LES, the numerical simulations are performed in cuboid computational domains that can be used to simulate the flame