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Numerical simulation of flame acceleration and deflagration-to-detonation transition of ethylene in channels

Cheng Wang [a], Yongyao Zhao [a], Bo Zhang [b, *]

[a] Beijing Institute of Technology, State Key Laboratory of Explosion Science and Technology, Beijing, 100081, China
[b] East China University of Science and Technology, Key Laboratory of Coal Gasification and Energy Chemical Engineering of Ministry of Education, Shanghai, 200237, China

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ABSTRACT

Ethylene (C_2H_4) is a hydrocarbon fuel and widely used in chemical industry, however, ethylene is highly flammable and therefore presents a serious fire and explosion hazard. This work is initiated by addressing the hazard assessment of ethylene mixtures in different scale channels ($d = 5$ mm, 10 mm and 20 mm) from the aspect of flame acceleration (FA) and deflagration-to-detonation transition (DDT) by using large eddy simulation (LES) method coupled with the artificially thickened flame (ATF) approach. The fifth order local characteristics based weighted essentially non-oscillatory (WENO) conservative finite difference scheme is employed to solve the governing equations. The numerical results confirm that flame velocity increase rapidly at the beginning stage in three channels, and the flame acceleration rate is slower in the subsequent stage, afterwards, the flame velocity has an abrupt increase, and the onset of detonation occurs. Due to the fact that wall effect is significant in the narrow channel (e.g.,5 mm), especially in the ignition stage of the flame, flames have different shapes in wider channels (10 mm and 20 mm) and narrow channel (5 mm). Both the pressure and temperature profiles confirm DDT run-up distances are 0.251 m, 0.203 m and 0.161 m in 20 mm, 10 mm and 5 mm channels, respectively, which indicates that a shorter run-up distance is required in narrower channel. The cellular detonation structures for the ethylene-air mixture in different channels indicate that multi-headed detonation structures can be found in 20 mm channel, as the channel width decreases to 10 mm, detonation has a single-headed spinning structure, as the width is further reduced to 5 mm, only large longitudinal oscillation of the pressure can be observed.

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1. Introduction

Ethylene (C_2H_4) is a hydrocarbon fuel and widely used in chemical industry, and whose worldwide production exceeds other organic compounds. However, ethylene is extremely flammable and therefore presents a serious fire and explosion hazard. For example, the flammability range of ethylene in air is 2.7%–36%. Ethylene-air mixture can be ignited by a hot surface without a flame or spark. Therefore, the key challenges in the widespread use of ethylene as an energy carrier are safety-related issues. Explosion and detonation hazards associated with the production, handling, transportation and storage of ethylene must be controlled with a minimized risk to society (Zhang and Bai, 2014; Zhang and Ng, 2015, 2016).

In general, most of the explosions of combustible gaseous mixtures (includes ethylene-air) start with an electrical spark or the auto-ignition in contact with a hot surface when the flame traveling in piping and reactors (Nie et al., 2014; Wang et al., 2014). The flame always accelerates and undergoes a transition to detonation along with a high pressure peak. In order to prevent and mitigate accidental explosions in production and storage, and control the detonation initiation in pulse detonation engines (PDE), it is necessary to investigate the mechanism of deflagration-to-detonation transition (DDT) and the detonation structures as well as the direct detonation initiation (Zhang et al., 2014; Zhang et al., 2013, 2012; Zhang et al., 2011; Zhang et al., 2011). A number of fundamental studies have been performed (Teng et al., 2014; Teng et al., 2015; Teng & Jiang, 2012, 2013) which are investigated through experiments, theoretical analysis, and numerical methods

* Corresponding author.
E-mail address: bzhang@ecust.edu.cn (B. Zhang).

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in recent years (Ciccarelli and Dorofeev, 2008; Dorofeev, 2011; Ivanou et al., 2011; Kagan and Sivashinsky, 2003; Thomas et al., 2010; Valiev et al., 2009). Previous studies have found that the behavior of DDT and the propagation of detonation in combustible mixtures would be different if the channel scale is changed (Gao et al., 2014; Wu et al., 2007; Wu and Wang, 2011). Wu et al., 2007 argued that the flame propagates in larger tubes always takes a longer distance to transmit to detonation. Bychkov et al., 2005 showed that the flame velocity grows faster in response to a decreasing Reynolds number (by decreasing the width of channel). The detonation propagation limits in the narrow gaps and channels were extensively examined by Zhang et al., 2016; Zhang et al., 2016; Zhang et al., 2015, 2016 recently. They explored the effect of detonation instability, the properties of mixture and the wall effect of the channel on the limits. In the wider channel, the run-up distance of DDT is longer and the detonation wave with multi-headed structure always propagates as Chapman-Jouguet (CJ) velocity. As the channel width decreased, multi-headed detonation disappears, instead, other detonation modes, e.g., double-headed and single-headed spinning, supported by complex interaction of shock compression and chemical reaction, are found from experimental observations (Camargo et al., 2010; Gao et al., 2015) and numerical simulations (Wang et al., 2013; Chinnayya et al., 2013; Huang et al., 2014; Kurosaka and Tsuboi, 2014).

For numerical simulation of detonation initiation and propagation in the combustible mixtures (includes ethylene-air), previous work focused on the Direct Numerical Simulation (DNS) method. However, DNS for the DDT process in laboratory scale is a formidable task in a three-dimensional geometry and even in a simple two-dimensional geometry. The mesh resolution requirements should be less than the smallest scales of chemistry and fluid mechanics, therefore the computation is very expensive. Because the DNS is highly improbable for large-scale DDT simulation, we are focusing on Large Eddy Simulation (LES) that is less expensive but has a good performance in simulating the flame acceleration (FA) and DDT. In this work, we also developed a parallel solver of the LES adopting a fifth-order weighted essentially non-oscillatory (WENO) scheme with a third-order TVD Runge-Kutta time stepping method is applied (Wang, C., Shu, C., Han, W., & Ning, J. 2013), for numerically investigate the DDT process and the detonation propagation behavior of ethylene-air mixture in different channels. The objective of this work is to provide a reliable numerical simulation method for studying the FA and DDT in ethylene-air, which is useful to quantitatively analyze the detonation characteristics of ethylene, and establish a better understanding of the FA and DDT behaviors.

2. Governing equations and numerical details

The governing equations are constructed by filtering the compressible instantaneous conservation Navier-Stokes equations for mass, momentum, total energy, and species conservation. The spatial filter for flow variable f is given by:

$$\overline{f}(x) = \int f(x')F(x-x')dx' \tag{1}$$

where the integral is over the entire flow domain and $F(x)$ is some filtering function. Here, we use a box filter based on local grid size Δ for the spatial filter. Then, the resulting LES equations are as follows by applying Favre averaging, which is defined by $\tilde{f} = \overline{\rho f}/\overline{\rho}$.

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_i}{\partial x_i} = 0 \tag{2}$$

$$\frac{\partial \overline{\rho}u_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}u_i u_j + \overline{P}\delta_{ij}\right) = \frac{\partial}{\partial x_j}\left(\tilde{\tau}_{ij\cdot}\right) - \frac{\partial}{\partial x_j}\left(\tau_{ij}^{sgs}\right) \tag{3}$$

$$\frac{\partial \overline{\rho}\tilde{E}}{\partial t} + \frac{\partial}{\partial x_i}\left(\left(\overline{\rho}\tilde{E} + \overline{P}\right)\tilde{u}_i\right) = \frac{\partial}{\partial x_i}\left(\tilde{u}_i\tilde{\tau}_{ij}\right) - \frac{\partial \overline{q}_i}{\partial x_i} - \frac{\partial}{\partial x_i}H_i^{sgs} \tag{4}$$

$$\frac{\partial \overline{\rho}\tilde{Y}}{\partial t} + \frac{\partial}{\partial x_i}\overline{\rho}\tilde{Y}\tilde{u}_i = \frac{\partial}{\partial x_i}\left(\overline{\rho}D_i\frac{\partial \tilde{Y}}{\partial x_i}\right) - \frac{\partial}{\partial x_i}\phi_i^{sgs} + \overline{\dot{\omega}} \tag{5}$$

here ρ,u,P,E and Y denote density, velocity, pressure, total energy and mass fraction respectively. Further, τ,q,D and $\overline{\dot{\omega}}$ are the stress tensor, energy diffusion vector, coefficient of mass diffusion and filtered reaction rates. Compared with DNS equations, the sub-grid scale (SGS) will appear at the right-hand side in the LES equations. The SGS stress τ_{ij}^{sgs}, the unclosed term H_i^{sgs} in the energy equation, SGS diffusion of specie mass fraction and SGS reaction rate are as following:

$$\tau_{ij}^{sgs} = -2\overline{\rho}\upsilon_t\left(\tilde{s}_{ij} - \frac{1}{3}\tilde{s}_{ij}\delta_{ij}\right) + \frac{2}{3}\overline{\rho}k^{sgs}\delta_{ij} \tag{6}$$

$$H_i^{sgs} = -\overline{\rho}\frac{\upsilon_t}{pr_t}\frac{\partial \tilde{h}}{\partial x_i} \tag{7}$$

$$\phi_i^{sgs} = -\overline{\rho}\frac{\upsilon_t}{Sc_t}\frac{\partial \tilde{Y}}{\partial x_i} \tag{8}$$

$$\overline{\dot{\omega}} = -A\overline{\rho}\tilde{Y}\exp\left(-\frac{Q}{R\tilde{T}}\right) \tag{9}$$

here $\upsilon_t = C_\upsilon(k^{sgs})^{1/2}\Delta$, k^{sgs} is the subgrid kinetic energy, and $h = E + P/\rho$ denotes total enthalpy. The one-equation model for k^{sgs} solved along with the LES equations is

$$\frac{\partial \overline{\rho}k^{sgs}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\tilde{u}_i k^{sgs}) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\frac{\upsilon_t}{pr}\frac{\partial k^{sgs}}{\partial x_i}\right) - \tau_{ij}^{sgs}\left(\frac{\partial \tilde{u}_i}{\partial x_j}\right) - C_e\overline{\rho}(k^{sgs})^{3/2}\Big/\Delta \tag{10}$$

Constants 0.067 and 0.916 are employed for C_υ andC_e, andPr_t, Sc_t are taken as 1.0.

In the LES method, the grid size is typically larger than the thickness of the flame front. In the ATF model, the flame is artificially thickened which can be resolved on the LES grid, which is simply achieved by decreasing the pre-exponential factor in the Arrhenius law. The thickening flame modifies the interaction between turbulence and chemistry, so the ratio of the turbulent and chemical time-scales named Damköhler number (Da) is also decreased by a factor F and becomes Da/F. When the Da decreases, the flame becomes less sensitive to turbulent motions. The subgrid scale effects have been considered to incorporate into the thickened-flame model and parametrized using an efficiency function E_F (Colin et al., 2000). Using the efficiency function, the final form of mass fraction equation (4) can be re-written as:

$$\frac{\partial \overline{\rho}\tilde{Y}}{\partial t} + \frac{\partial}{\partial x_i}\overline{\rho}\tilde{Y}\tilde{u}_i = \frac{\partial}{\partial x_i}\left(\overline{\rho}E_F F D_i\frac{\partial \tilde{Y}}{\partial x_i}\right) - \frac{\partial}{\partial x_i}\varphi_i^{sgs} + \frac{E_F\overline{\dot{\omega}}}{F} \tag{11}$$

In this study, we use a dynamic TF approach (Durand and Polifke, 2007). The thickening factor is based on the mass fraction and defined as $F = 1 + (F_0 - 1)\Omega$, where F_0 is set to $max\,(N\Delta/\delta_L, 1)$, N is the grid number in the flame front, Δ is the cell size andδ_L is the

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