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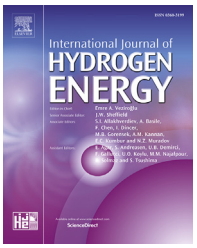

Numerical study of hydrogen–oxygen flame acceleration and deflagration to detonation transition in combustion light gas gun

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ABSTRACT

A large eddy model with detailed chemical reaction mechanism is developed to investigate the interior ballistic process of the combustion light gas gun (CLGG). Flame acceleration and deflagration to detonation transition process with high initial pressure and low initial temperature hydrogen–oxygen mixture in CLGG is numerically studied. Simulation results indicate that the hydrogen–oxygen flame propagation experiences an exponential acceleration stage, a nearly uniform propagation stage and a fast reacceleration stage. Detonation can be triggered through two different mechanisms, which are the amplification between the overlapped shock wave at flame surface, and the elevated flame velocity and shock strength caused by local explosions. Reflected shock waves play an important role in the suppression of the flame propagation when the flame front is close to the chamber throat, leading to a deceleration of the deflagration flame.

Introduction

The Combustion Light Gas Gun (CLGG) is an advanced launching system with extremely high muzzle velocity, of which the projectile is propelled by the combustion expansion of low molecular weight combustible gas mixture. It is shown that the muzzle energy provided by this technique is at least 30% higher than that obtained from advanced solid propellant guns [1], which makes an obvious advantage on the cannon range and the launching load. Generally, the propelling charge in CLGG is hydrogen–oxygen mixture with high loading density, which, under certain conditions, will accelerate to fast deflagration in a very short period of time after ignition. Thus, it is essential to carry out research on the relevant hydrogen–oxygen flame acceleration and deflagration to detonation transition (DDT) in the interior ballistic process of CLGG, so as to avoid the safety accidents in experiment.

The research attempts to clarify the DDT mechanism has a long history that begins with Zel'dovich et al. [2], the principle of Zel'dovich gradient mechanism is that flame velocity is determined by the gradient of induction time when a spontaneous reaction wave travels through a reactive gas mixture with uneven heat distribution, which is not limited by the local sound speed and the reaction wave may evolve into a sustained detonation wave. Lee and Moen [3] proposed a similar explanation which is known as the shock wave amplification through coherent energy release (SWACER) theory. They believe that when a spontaneous reaction wave propagates through a reactive mixture with a gradient of chemical induction time at a velocity roughly between the Chapman–Jouguet velocity and the local speed of sound, it

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may develop into a self-sustained detonation wave due to the strong positive feedback between the chemical energy release and the shock wave it generates.

Later, a number of numerical and experimental studies are carried out to investigate the spatio-temporal formation mechanism of the hot spots and the origin of DDT. Khokhlov [4,5] simulated the flame acceleration and DDT in a smooth tube with mesh grids processed by self-adaptation optimization method based on fully threaded tree theory, their numerical work reproduced the wrinkling process of flame front via the Richtmyer-Meshkov instability and the formation process of hot spots due to the pressure fluctuations generated by shock–flame interactions. Oran and Gamezo [6] pointed out that shockwaves propagating nearby flame front strengths the turbulent fluctuation of the unreacted mixture, which in turn enhances the thermal exchange and the species transport of this area. They concluded that turbulence does not trigger DDT directly, but creates conditions for germination of hot spots at the vicinity of the flame brush. Kuznetsov [7,8] proposed that the turbulent fluctuation deeply affected by the boundary layer in a smooth narrow tube is propitious to form small scale nonuniformity near the flame, which may leads to a spontaneous wave with extremely high velocity (above C-J detonation velocity) and triggers the detonation.

The LES research of Yongyao Zhao [9] indicates that flame in a small scale smooth tube may keep accelerating in laminar condition until DDT occurs. Local explosion caused by the intersection of complex shock waves near the wall is believed to be the trigger of detonation transition. The research of Dziemińska [10] shows that auto-ignition of the preheat unburnt mixture within the boundary layer caused by shock-boundary layer interaction may accelerate into a supersonic flame due to the shock driven effect from the original flame surface and then evolves into the final detonation. Akiki [11] analyzed the physical and chemical dynamics of the DDT process triggered by the stimulating effect of an intense shock to hot-spots. Liberman et al. [12,13] numerically studied the temperature gradient scale capable to initiate detonation, and found that the single-step reaction model will give a lower prediction on the reaction induction time, which leads to an error prediction on the minimal length of the temperature gradient capable to trigger detonation. To remedy the defect, a detailed or simplified multi-step reaction model with necessary chain branch reactions is highly recommended. It is believed that the DDT mechanism is different from the widely accepted Zel'dovich gradient mechanism and should be interpreted as the strong amplification between reaction heat release and the shock wave when they are overlapped and propagating together. The numerical study of Ivanov et al. [14–16] shows that the flame acceleration process in small-scale smooth tubes can be divided into 3 distinct stages, which are (1) Flame accelerates exponentially with weak pressure waves generated, (2) flame acceleration nearly frozen with shock waves rising and growing stronger ahead of the flame, (3) shock waves overlapped with flame surface and strengthen exponentially with velocity increasing explosively until DDT occurs.

Our previous numerical research of the interior ballistic process of CLGG [17,18] was mainly based on the RANS model and EDM combustion model. This model may simulate the interior ballistic process reasonably with coarse mesh, but will give a poor prediction of the laminar flame in the initial stage, and is unable to reproduce the DDT process. This paper presents a relatively high temporal and spatial resolution LES with detailed elementary chemical reaction model for the simulation of the interior ballistic process of CLGG. The high pressure hydrogen–oxygen flame acceleration process under different initial component ratios is studied; the relevant two different DDT processes are analyzed.

Mathematical model

Flow variables in the LES model are decomposed into mean and fluctuating parts by the filtration scale, which represents the delegate the large-scale vortex and small-scale fluctuations respectively. The abstracted large-scale average quantity is directly solved by the corresponding governing equations, while the small-scale fluctuations are modeled by the sub-grid scale (SGS) model. For compressible flow, the governing equations with Favre-averaged quantities can be written as:

1) Mass conservation equation:

$$\frac{\partial}{\partial t}(\overline{\rho}) + \frac{1}{r}\frac{\partial}{\partial x_j}(r\overline{\rho}\tilde{u}_j) = 0 \tag{1}$$

2) Momentum conservation equation

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{u}_i) + \frac{1}{r}\frac{\partial}{\partial x_j}(r\overline{\rho}\tilde{u}_i\tilde{u}_j) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{1}{r}\left(\frac{\partial}{\partial x_j}\left(r\mu\tilde{S}_{ji}\right) - \delta_{2i}\left(\frac{2}{3}\mu\nabla\vec{V}el - 2\mu\frac{\tilde{v}}{r}\right)\right) - \frac{1}{r}\frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

3) Species conservation equation

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{Y}_k) + \frac{1}{r}\frac{\partial}{\partial x_j}(r\tilde{u}_j\tilde{Y}_k) = \frac{1}{r}\frac{\partial}{\partial x_j}\left(r\left(D_k\frac{\partial \tilde{Y}_k}{\partial x_j} + Y_k^{SGS} + S_k^{SGS}\right)\right) + \overline{\dot{\omega}}_k \tag{3}$$

4) Energy conservation equation

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{e}) + \frac{1}{r}\frac{\partial}{\partial x_j}(r\overline{\rho}\tilde{u}_j\tilde{h}) = \frac{1}{r}\frac{\partial}{\partial x_j}\left(r\frac{K}{c_p}\frac{\partial \tilde{h}}{\partial x_j} - \frac{\partial Q_i}{\partial x_j}\right) + \tilde{u}_j\frac{\partial \overline{p}}{\partial x_i} + \left(\tilde{u}_j\tilde{S}_{ji} - \tau_{ij}\right)\frac{\partial \tilde{u}_i}{\partial x_j} + S_{energy} \tag{4}$$

In the above equations ρ, u_i, p, δ_{ij}, Y_k and $\dot{\omega}_k$ represent density, velocity component, pressure, Kronecker delta, mass

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