Flame acceleration and deflagration-to-detonation transition in micro- and macro-channels: An integrated mechanistic study

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ABSTRACT

The integrated processes of flame acceleration, deflagration-to-detonation transition (DDT), and the resulting detonation propagation in micro- and macro-scale channels are simulated. It is found that the modes of flame acceleration and DDT in these two channels are different, being primarily controlled by viscosity and turbulent flame development, respectively. Furthermore, while boundary layer ignition is crucial for DDT in both channels, viscous wall friction is the key to self-sustained propagation in micro-channels, leading to momentum loss and consequently deficit of the detonation velocity. In macro-channels, the strong overdriven detonation decays and gradually evolves into the Chapman–Jouguet detonation.

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1. Introduction

Deflagration-to-detonation transition (DDT) in channels is believed to involve the acceleration of a low-speed laminar flame from a weak ignition source to a high-speed deflagration wave through various processes which would trigger local explosions and eventually transition to detonation. Understanding the entire transition process not only is of fundamental significance, but it also commands practical interests such as mitigation of explosion hazards and the development of pulse-detonation engines [1,2].

Previous studies on DDT in channels with relatively large widths, for example $O(10\,\text{mm})$ and larger, have shown that the development and interaction of turbulent flames, shocks, hot spots and reaction gradients [3–8] are essential in the transition to detonation [9]. Urtiew & Oppenheim and Meyer & Oppenheim [10,11] clearly observed DDT, and found that the transition modes depend on the interaction of the wave appearing ahead of the accelerating flame. Valiev, Bychkov and Akkerman et al. [6] showed theoretically that compressibility of the gas moderates the flame acceleration. Liberman and Ivanov et al. [7] presented experimental studies of DDT in highly reactive hydrogen–oxygen and ethylene–

oxygen mixtures, and showed that viscous friction from no-slip walls is the key factor of the origin of DDT. Gamezo, Khokhlov and Oran [12] examined numerically the effects of bifurcated shock structure on shock–flame interaction and ethylene–air DDT in shock-tube experiments. Their results showed that the presence of bifurcated structure leads eventually to hot spots behind the Mach stem, thus facilitating DDT. Zel'dovich [8] discussed the propagation velocity of the reaction wave in the mixture with nonuniform initial conditions, and showed that the reaction gradient triggers the DDT. Liberman et al. [13] studied the formation of the preheated zone ahead of a propagation flame and the sequential reactivity gradient, considered as a mechanism underlying the DDT.

Furthermore, numerical studies [10,12–15] suggested that viscosity could affect the DDT distance, the detailed transition mechanism [6,7,9,13,15], as well as propagation of the generated detonation [14,16–19]. These simulations, however, were conducted separately for the isolated phases of laminar flame acceleration [9,20], turbulent flame evolution and DDT [2,12], and the propagation of directly initiated detonations [18,19,21]. For example, Bykov et al. [14] showed theoretically that hydraulic resistance and heat loss affect the detonability and flammability limits; the shock bifurcation observed by Gamezo et al. [12] results from the boundary layer induced by viscosity; the origin of DDT is relevant to the interaction of shock with boundary layer [4,7]; and the experimental observation of detonation propagation in tubes with porous wall

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[21], leading to the understanding that the drag from the porous wall leads to velocity deficit.

As the channel width is reduced to the micro-scale, defined by Wu et al. [5], effects of viscosity and heat transfer from the wall become more significant [4,5,9,15,19,22,23], as is reasonable to expect. The ensuing laminar flame accelerates and eventually transitions to detonation through thermal explosion in the wall boundary layer [16]. Consequently viscous effects directly affect the transition, while the associated viscous loss could also lead to reduction of the detonation velocity from the CJ value [5,20,21]. Kagan and Sivashinsky [15] discussed the important role of hydraulic resistance in DDT in a thin, semi-infinite and thermally-insulated channel. Brailovsky and Sivashinsky [4] also found that DDT was triggered by localized thermal explosion in the extended preheat zone induced by wall friction. Wu et al. [5,22] observed the occurrence of DDT through experiments in the micro-scale channel (0.25–3.0 mm) filled with ethylene–oxygen mixture, and found deficit in the detonation velocity. Furthermore, Ishii, Itoh and Tsuboi [19] experimentally studied the detonation velocity deficits in narrow gaps due to viscous drag. Studies of the combustion waves in hydraulically resisted systems were reviewed by Brailovsky et al. [16].

Recognizing the complexity and highly-coupled nature of the individual processes leading to DDT and the subsequent detonation propagation, the potential role of viscosity with varying channel dimension, and that an *integrated* study of the individual processes has not been undertaken, in the present investigation we have simulated the entire process of DDT, from initiation by an ignited flame to the subsequent detonation propagation, in micro- and macro-channels, by solving the system of reactive conservation equations including the Navier–Stokes (NS) equations. Consequently we are able to identify the specific mechanisms of DDT and the subsequent detonation propagation mode in these channels of highly disparate dimensions, when subjected to viscous action. Furthermore, we shall identify the respective roles of pulsation and cellular instabilities as well as the early burning in front of the turbulent flame in the DDT processes.

2. Governing equations and numerical methods

The conservation equations including the compressible NS equations, with advection, diffusion and reaction sources, are given by

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j + \delta_{ij}p - \zeta_{ij}) = 0, \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho e + \frac{1}{2}\rho u_i u_i\right) + \frac{\partial}{\partial x_j}\left(\rho u_j h + \frac{1}{2}\rho u_i u_i u_j + \sigma_j - u_i \zeta_{ij}\right) = 0, \tag{3}$$

$$\frac{\partial(\rho Y)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i Y - \frac{\mu}{Sc}\frac{\partial Y}{\partial x_i}\right) = -A\rho Y \exp(-E_a/R_p T), \tag{4}$$

$$p = \rho R_p T/M. \tag{5}$$

Here ρ, p, u and T are the density, pressure, velocity and temperature, respectively, Y is the mass fraction of the multicomponent gas, $e = QY + C_V T = QY + R_p T/(\gamma-1)$ the internal energy, and $h = QY + C_p T = QY + R_p T\gamma/(\gamma-1)$ the enthalpy, which are all functions of space x and time t. Furthermore, Q is the heat of reaction, C_V and C_p the specific heats at constant volume and constant pressure, respectively, R_p the ideal gas constant, M the molar mass, γ the adiabatic exponent, and E_a and A the activation energy and pre-exponential factor of the assumed one-step overall reaction, respectively. The stress tensor ζ_{ij} and the energy diffusion vector σ_j are respectively given by

$$\zeta_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right), \tag{6}$$

$$\sigma_j = \mu\left(\frac{C_p}{Pr}\frac{\partial T}{\partial x_j} + \frac{Q}{Sc}\frac{\partial Y}{\partial x_j}\right). \tag{7}$$
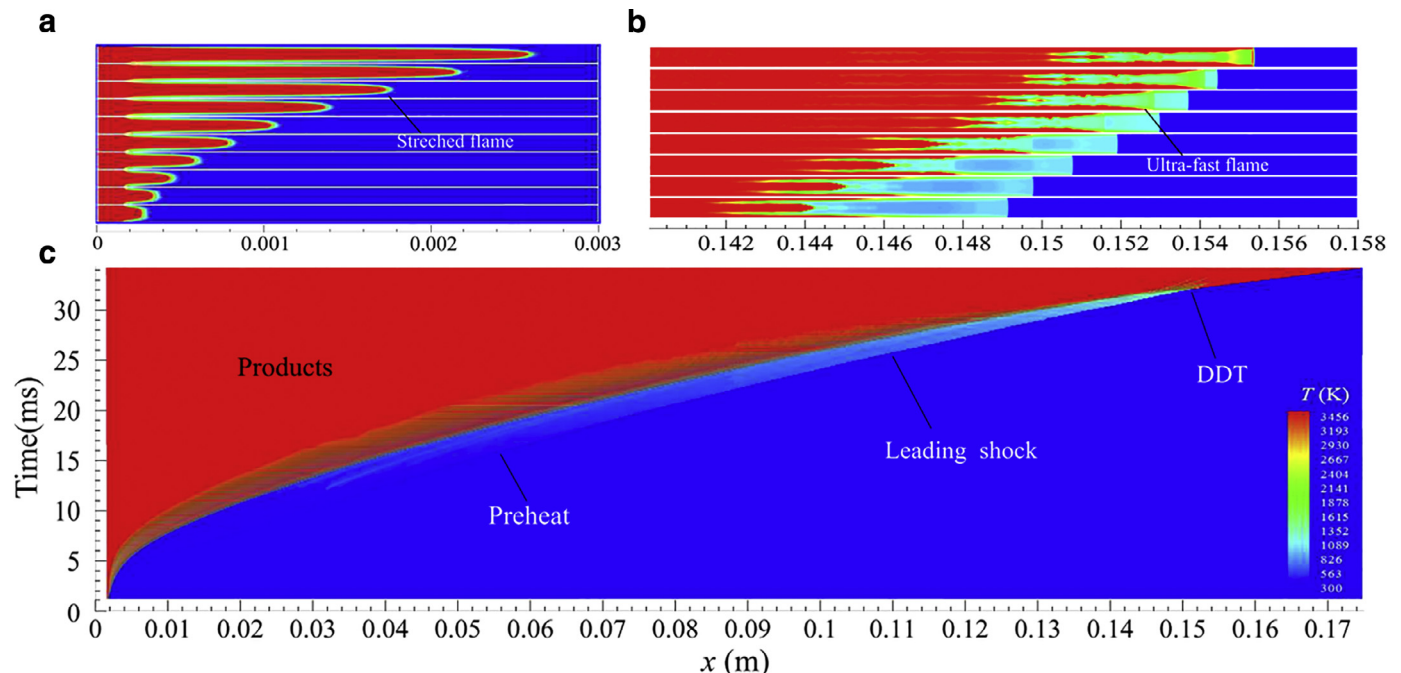

Fig. 1. Flame acceleration, DDT and detonation in the micro-channel: (a) Exponential acceleration; (b) DDT; (c) Entire process of DDT including the exponential and linear acceleration and the transition to detonation. (a) and (b) are the locally zoomed segments of (c).