Flame Acceleration and Transition to Detonation in Methane-air Mixtures with Composition Gradients

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1 Introduction

Deflagration-to-detonation transition (DDT) is an important topic for safety in industrial environments [1,2] and optimizing propulsion devices [3,4]. There has been many research for hydrogen-air mixtures with composition gradients. These include experimental studies of the influence of mixture inhomogeneity on flame acceleration [5], DDT [6], and detonation propagation [7,8] in both smooth and obstructed channels. There are also numerical simulations of these experiments [9,10] that have provided further understanding of DDT in obstructed channels. These studies showed that inhomogeneous mixtures are more likely to undergo DDT than homogeneous mixtures when the average equivalence ratios are in the fuel-lean regime.

In comparison, relatively little is known about the influence of mixture inhomogeneity on the explosion procedure for methane-air mixtures (e.g., [11-13]). Kessler et al. [14] numerically studied detonation propagation through inhomogeneous methane-air mixtures in smooth channels in which the composition gradients were aligned perpendicular to the propagation direction of the reaction wave. This work showed that detonations propagate more slowly for steeper gradients and are quenched when the gradients are large enough [14]. Zheng et al. [15] recently addressed a similar problem in a two-dimensional, obstructed channel with a methane-air mixture in which the composition gradient varied linearly from the lean detonation limit at the bottom of the channel to the rich detonation limit on the top. The results showed that the flame speed is smaller and the transition to detonation is delayed in the inhomogeneous mixture compared with the stoichiometric, homogeneous case.

This paper is part of a more comprehensive study of the effect of composition gradients on flame acceleration and DDT in methane-air mixtures. Here, we present four cases with two linear distributions and two nonlinear distributions of composition gradients. In all cases, the gradients are both perpendicular to

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the main direction of reaction propagation. The problem is addressed numerically by solving the unsteady, fully compressible, reactive Navier-Stokes equations. The solution method uses a calibrated, optimized chemical-diffusive model (CDM) that reproduces correct flame and detonation properties for methane-air mixtures over a range of equivalence ratios [16,17]. The new CDM model was previously validated for homogeneous methane-air mixtures and then applied to the calculation of DDT in an inhomogeneous methane-air mixture [15]. Now it is used to study the effect of several different composition gradients in mixtures of methane and air. The physical and numerical model used in this paper is the same as that in [15].

2 Numerical Setup

The computational setup describes a two-dimensional channel with uniformly spaced obstacles, shown in Fig.1, which is similar to the experimental system of Kuznetsov et al. [11]. The channel is closed at the left end ($x = 0$) and open to the atmosphere at the opposite end ($x = L$). We assume a nonslip, adiabatic wall at the bottom plane ($y = 0$) and the left boundary ($x = 0$), as well as the face of every obstacle. A zero-gradient outflow boundary condition is imposed at the open end on the right side, and the initial gas is 1 atm and 293 K throughout the channel. A symmetry condition is applied to the top boundary. To ignite the flame, we place a semi-circular region of hot, burned material of 1 atm and 3000 K at the center of the left boundary. Initial distributions of composition gradients in the y-direction of the channel for the four inhomogeneous cases studied in this paper, $\phi = 0.5 - 1.5$, $\phi = 1.5 - 0.5$, $\phi = 0.5 - 1.5$_G1, $\phi = 0.5 - 1.5$_G2, are shown in Fig.2. The grid resolution used in this paper is the same as that in [15], which has been tested for both homogeneous and inhomogeneous methane-air mixtures and shown to resolve flames, shocks, boundary layers, and other important flow and chemical structures, given the new CDM model discussed above.

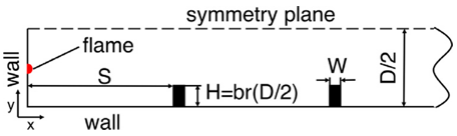

Figure 1: Computational setup. $D = 0.174\,\mathrm{m}$, $H = 2.61 \times 10^{-2}\,\mathrm{m}$, $S = 0.174\,\mathrm{m}$, $W = 2 \times 10^{-2}\,\mathrm{m}$, $L = 11.878\,\mathrm{m}$. Blockage ratio $br = 0.3$. Initial flame radius is $2.5 \times 10^{-3}\,\mathrm{m}$.

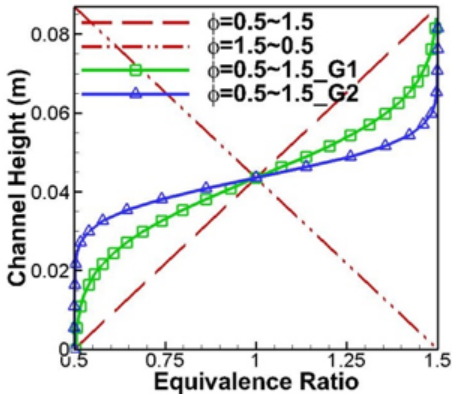

Figure 2: Initial distributions of equivalence ratios over the channel height for inhomogeneous cases.

3 An Overview

Fig.3 gives an overview of the temperature at the leading edge of the flame for one of the gradients considered. The figure allows us to compare the results in the homogeneous mixture at equivalence ratio $\phi = 1.0$ and an inhomogeneous case in which the equivalence ratio linearly varies from $\phi = 0.5$ at the bottom of the channel to $\phi = 1.5$ near the top. During the initial stage of laminar flame expansion in the inhomogeneous mixture (rows 1-2), the flame expands more slowly and shows less wrinkling and a lower flame temperature, especially in the fuel-lean region near the bottom of the channel. As the flame becomes turbulent (rows 3-4), there are temperature gradients inside the flame and increased flame surface area between obstacles. The distance from ignition to the formation of a well-defined shock wave is greater in the inhomogeneous mixture than that in the homogeneous mixture (5th row).

The DDT process in inhomogeneous mixtures is qualitatively similar to that was reported for the detonation ignition in homogeneous mixtures in obstructed channels, which is through the Zeldovich gradient mechanism [18,19]. Here, a Mach stem becomes strong enough and reflects from the base of the obstacle, a hot spot forms at $x = 5.03\,\mathrm{m}$ (6th row), but fails to produce a detonation. The result is a shock and a flame at the base of the obstacle (7th row). A second hot spot eventually develops and transitions into a detonation at $x = 5.2\,\mathrm{m}$ (rows 8-10). The distance to DDT is greater in the inhomogeneous mixture than that in the homogeneous mixture at $x = 3.98\,\mathrm{m}$.

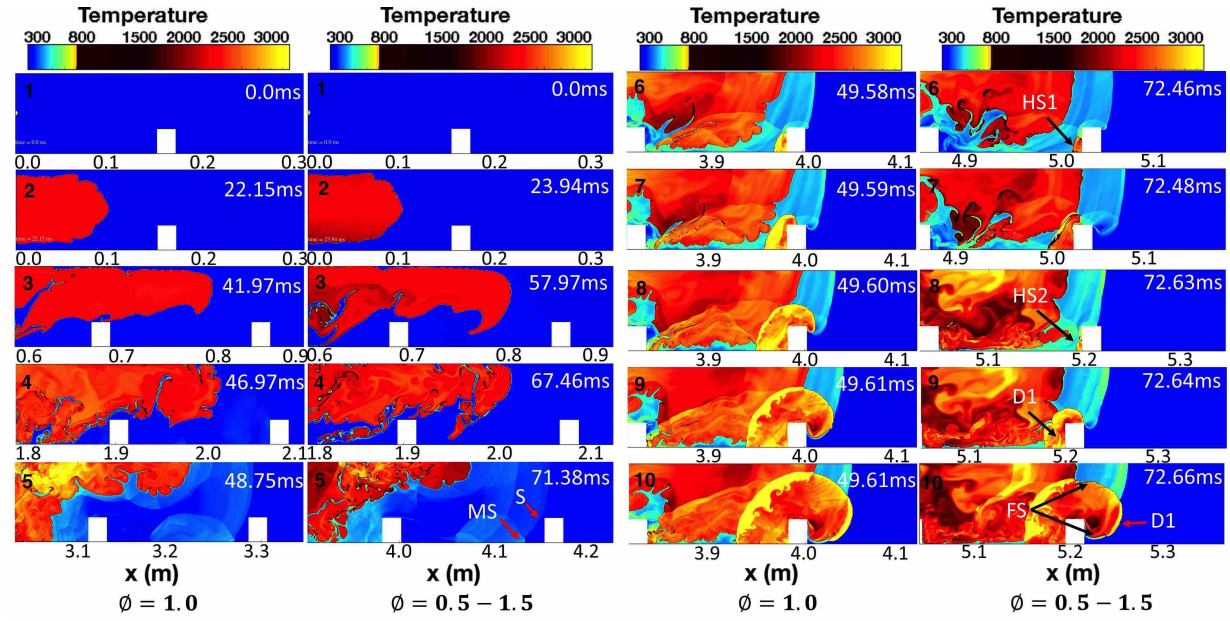

Figure 3: Temperature maps near the leading edge of the flame. Times and row numbers are shown in the frame corners. S - shock, MS - Mach stem, HS - hot spot, D - detonation, FS - flame surface.

4 Effect of Composition Gradients

Fig.4 shows the flame velocity, flame surface area, and total heat release as a function of the position of the leading edge of the flame. The flame accelerates more slowly in the inhomogeneous cases, and transitions

later to detonation. This results from the lower total heat release throughout the entire process, although the flame surface area is larger. This apparent contradiction was discussed in previous research [15]. It is explained by the low local heat release from the increased flame surface area.

The evolution of flame velocities (Fig.4a) calculated for the two inhomogeneous cases with linear composition gradients, $\phi = 0.5-1.5$ and $\phi = 1.5-0.5$, are very similar. This corresponds to the very similar trends for the total heat release (Fig. 4c), although the maximum flame surface area calculated for the $\phi = 0.5-1.5$ case is larger than that for the $\phi = 1.5 - 0.5$ case (Fig. 4b). As the composition gradient is steepened from $\phi = 0.5 - 1.5$_G1 to $\phi = 0.5 - 1.5$_G2, the flame velocity gradually decreases and is followed by a later transition to detonation (Fig.4a). The maximum flame surface area becomes larger (Fig.4b), and the total heat release becomes smaller (Fig. 4c). Fig.5 shows temperature and equivalence ratio maps near the reaction front during turbulent flame acceleration and formation of hot spots. The reasons for the above trends are complex and will be explained and presented in a longer paper.

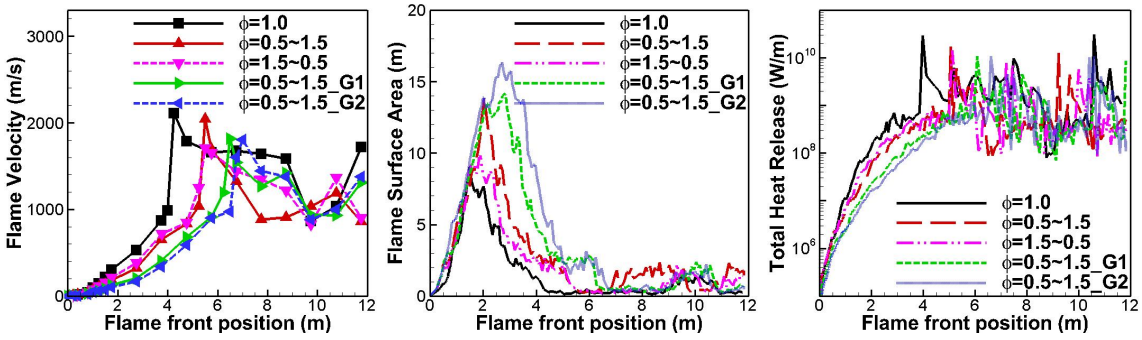

Figure 4: Left: flame velocity; middle: flame surface area; right: total heat releaseas a function of the position of the leading edge of the flame.

5 Conclusion

Unsteady, fully compressible numerical simulations of the evolution of ignition in inhomogeneous mixtures of methane and air in an obstructed channel were performed to investigate the effect of various composition gradients on the flame acceleration and DDT process. The new chemical-diffusive model is used to describe the chemical reactions with energy release, thermal conductivity, and molecular diffusion processes. The results show that the evolutions of flame velocity and total heat release are very similar for two inhomogeneous cases with reverse composition gradients. As the composition gradient is steepened, the maximum flame surface area increases and is reached at a longer distance. In this case, the distance to DDT also increases, resulting from the lower total heat release throughout the entire process.

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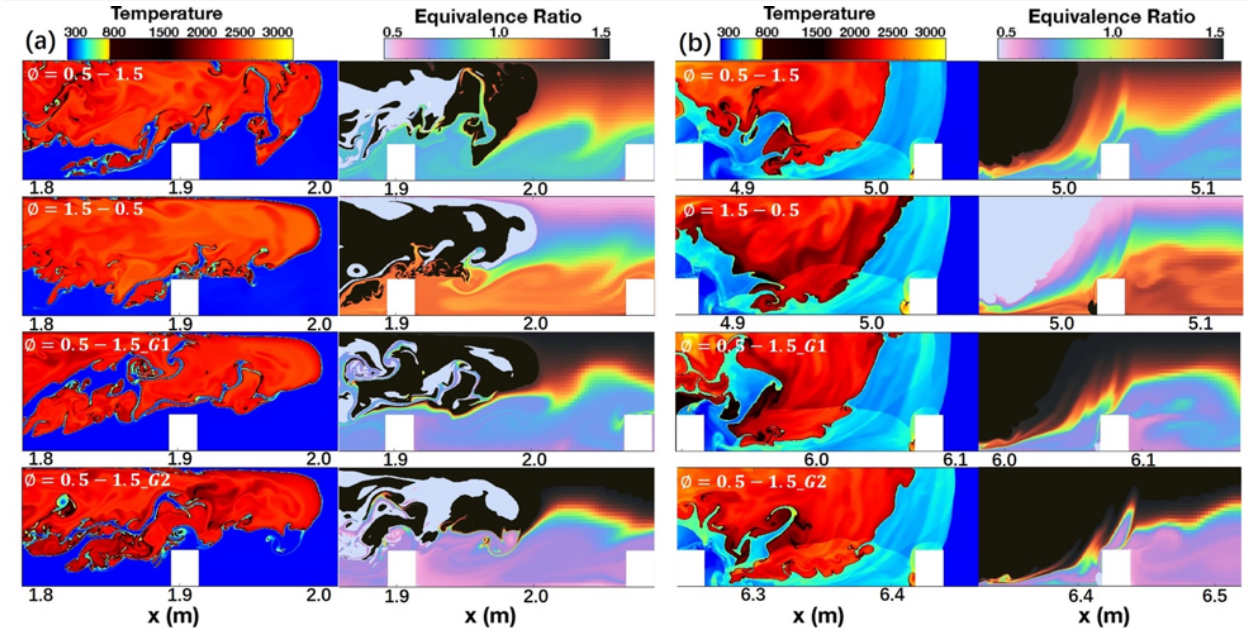

Figure 5: Temperature and equivalence ratio maps of the reaction front (a) during turbulent flame acceleration, and (b) formation of hot spot.

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