Numerical Study of Deflagration-to-Detonation Transition in Homogenous and Inhomogeneous Hydrogen-Air Mixtures

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Abstract

Explosions in homogeneous reactive gas mixtures have been widely studied both experimentally and numerically. However, in accident scenarios, combustible mixtures are usually inhomogeneous. The present numerical investigation aims to study flame acceleration and transition to detonation in homogeneous and inhomogeneous hydrogen-air mixtures with two different average hydrogen concentrations in a horizontal obstructed channel, filled with hydrogen-air mixture. A density-based solver was implemented within the OpenFOAM CFD toolbox. The Harten–Lax–van Leer–Contact (HLLC) scheme was used for accurate shock capturing. The numerical model initially has been verified by Sod's shock tube problem [1]. A high-resolution grid is provided by using adaptive mesh refinement, which leads to 30 grid points per half reaction length (HRL) in the finest regions near the flame and shock fronts. In agreement with the experimental measurements and observations, it was found that transverse concentration gradients lead to stronger flame acceleration and promote the transition to detonation for an average hydrogen concentration in air of 20%, whereas gradients slightly retard both phenomena for a 30% mixture.

1. Introduction

Thomas [3] gave a comprehensive discussion on various forms of deflagration-to-detonation transition (DDT) and differentiated the terminology between global DDT and local DDT. Global DDT includes the processes of flame acceleration (FA) and the onset of detonation. Local DDT refers to the actual onset of

detonation at the point where the combustion character changes from diffusion-controlled to auto-ignition controlled. In this work, the term DDT is used in the global sense and includes both FA and the onset of detonation.

While DDT in homogeneous mixtures has been widely investigated [4], the effect of spatial gradients in mixture composition has been studied less extensively. Kuznetsov et al. [5] conducted large-scale experiments of FA and DDT in an obstructed semi-confined flat layer of hydrogen–air mixture with transverse concentration gradients. It was suggested that DDT propensity in semi-confined mixtures with concentration gradients might be determined by the maximum local hydrogen concentration for globally lean mixtures. Vollmer et al. [6] and Boeck et al. [7,8,9] reported a strong effect of concentration gradients on FA and DDT in an entirely closed channel at laboratory-scale. However, Boeck et al. observed that in obstructed geometries, only in lean mixtures with an average hydrogen concentration below about 24%, concentration gradients promote FA and DDT, whereas for richer mixtures the presence of gradients leads to weaker FA and retards DDT. The authors suggested that a mixture-averaged analytical model for flame speed (σS_L) can predict differences in FA. For unobstructed channels, gradients always led to stronger FA and earlier DDT, independent of the average hydrogen concentration, due to flame surface area enlargement driven by spatial gradients in flame speed. The present work numerically investigates four cases that have been studied experimentally by Boeck et al. [2].

2. Numerical Approach

For numerical modelling, a density-based numerical code was developed [10] based on the OpenFOAM computational fluid dynamic (CFD) toolbox [11]. To evaluate the convective fluxes contribution, Harten–Lax–van Leer–Contact (HLLC) scheme with multidimensional slope limiters ("cellMDLimited" [12]) is used for accurate shock capturing. Compressible Navier–Stokes equations with a flame wrinkling combustion model are solved [12]. For turbulence modelling the Large Eddy Simulation (LES) technique with one eddy equation subgrid scale model is adopted. Also, the flame-wrinkling LES combustion model using conditional filtering, based on Weller et al. [12], has been implemented in the numerical code [13,14]. The solver and numerical schemes were initially tested by solving the Sod's shock tube problem [1].

3. The experiments considered

Previous experiments of Boeck et al. [2] of DDT in homogeneous and inhomogeneous hydrogen-air mixtures are modelled. The experiments were conducted in a horizontal partially obstructed channel. As shown in Figure 1, the channel was 60 mm high, 300 mm wide and 5.4 m long. Seven flat-plate obstacles with a blockage ratio of 60% were placed in a region 0.25 m<x<2.05 m from the ignition location at one end of the channel with an obstacle spacing of 0.3 m. The remaining channel length was unobstructed. Ignition was performed by a weak electric spark centered at x=0 m. Flame tip velocity was measured by photodiodes. As shown in Figure 2, concentration gradients were generated by gas injection through the channel top plate and subsequent diffusion. The gradients were oriented vertically, thus perpendicular to the main direction of flame propagation. In the present study four experimental cases are considered: (1) a homogenous mixture of 30% hydrogen in the air; (2) an inhomogeneous mixture of 30% hydrogen; (3) a homogenous mixture of 20% hydrogen; (4) an inhomogeneous mixture of 20% hydrogen.

4. Numerical setup

The computational domain represents the experimental geometry shown in Figure 1. Initial conditions are ambient pressure (101.325 kPa) and temperature (293 K). To mimic weak spark ignition, a patch of cells with a radius of 10 mm around the point of ignition (x=0 m, y=0.03 m) were set to a temperature of 2300

K at initial pressure. Two-dimensional simulation has been carried out. Adaptive mesh refinement provided a minimum cell size of 10 μm, resulting in approximately 30 grid points per half-reaction length in regions near the flame and shock fronts.

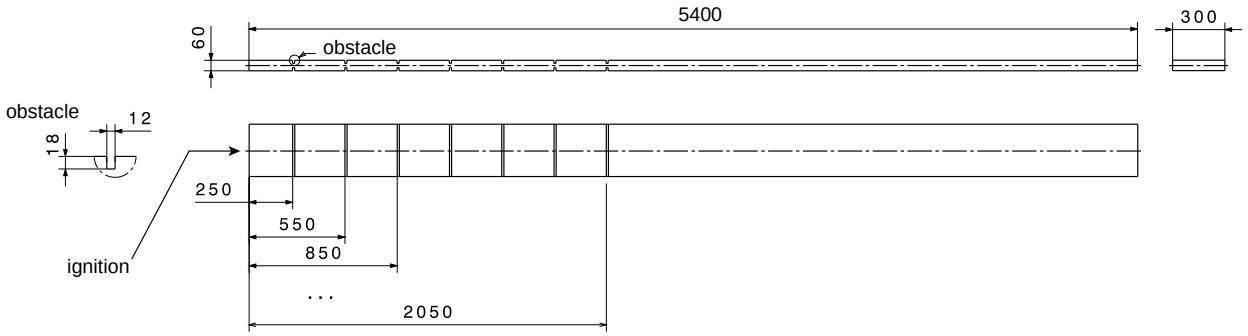

Figure 1. Geometry of the explosion channel. Dimensions in (mm).

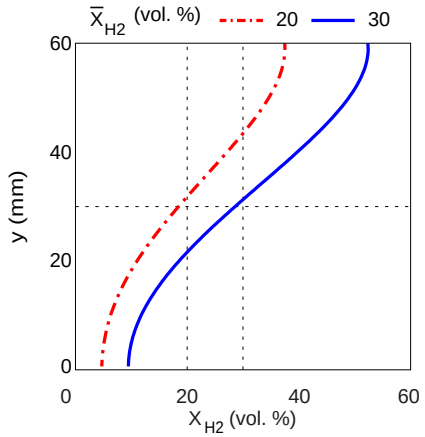

Figure 2. Hydrogen concentration profiles of inhomogeneous mixture cases 2 and 4.

5. Results and discussion

4.1 30% hydrogen (near-stoichiometric mixture)

As shown in Figures 3, the predicted flame tip velocities are in reasonably good agreement with the measurements. For both the homogeneous and inhomogeneous mixtures, the flame tip velocity rises continuously in the obstructed part of the channel. FA is slightly stronger in the homogeneous mixture. In accordance with the experiments [2,7], the transition to detonation is initiated by precursor shock reflection at the upstream faces of an obstacle, leading to local explosions behind the reflected shock wave and the onset of detonation either directly from the local explosions or from secondary hot-spots downstream of the obstacle. In the homogeneous mixture onset of detonation occurs between the obstacles located at x=0.85 m and x=1.15 m, whereas the onset takes place at the obstacle at x=1.45 m in the inhomogeneous mixture. Figure 4 shows pressure fields and numerical schlieren images (magnitude of the density gradient) of the onset in the inhomogeneous mixture. Experiments show a velocity deficit of detonation in the inhomogeneous mixture, discussed in more detail in [9]. Pressure transducers yield more accurate velocity data in the detonation regime than photodiodes (yellow and green markers). This effect of concentration gradients is not captured by the numerical simulations.

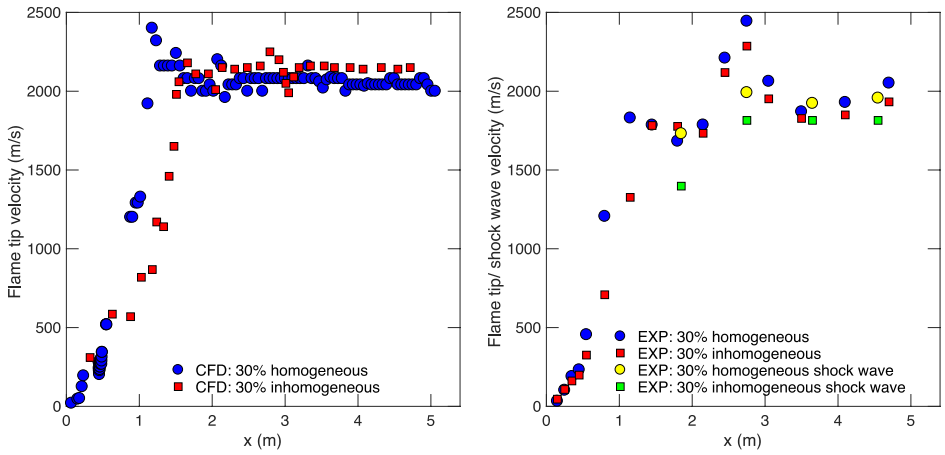

Figure 3. Comparison between flame tip velocities in homogeneous and inhomogeneous mixtures at 30% average hydrogen concentration; CFD (left) and experiments (right).

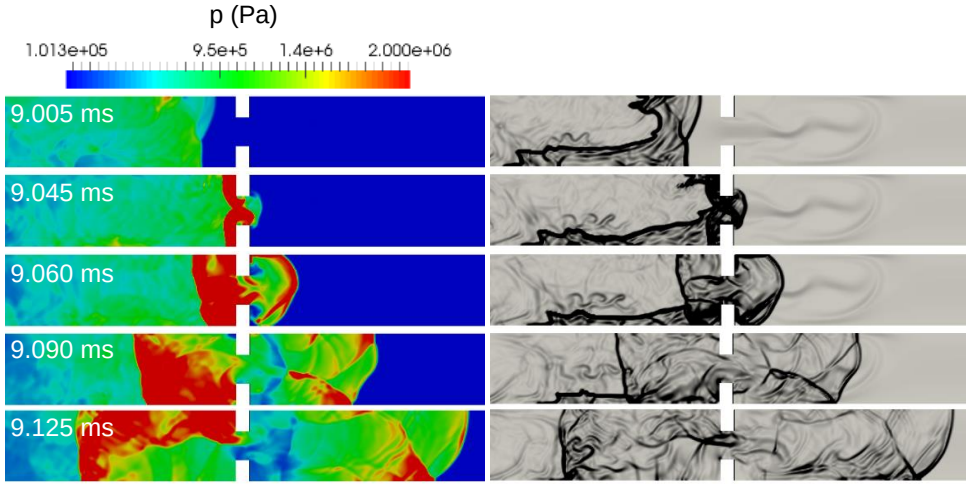

Figure 4. Pressure (left) and numerical schlieren (right, magnitude of density gradient) fields of detonation onset in the inhomogeneous 30% hydrogen-air mixture. The obstacle in the FOV is located at x=1.45 m.

4.2 20% hydrogen (lean mixture)

In contrast to the 30% hydrogen cases, FA is stronger in the inhomogeneous mixture for a 20% global hydrogen concentration as shown in Figure 5. The difference is small but measurable in the obstructed channel section. In the unobstructed section, the flame speed plateaus in the homogeneous mixture, whereas it keeps increasing in the inhomogeneous case. This steady acceleration in the unobstructed channel section in the inhomogeneous mixture was attributed to continuous enlargement of the flame surface area due to the concentration gradient [7,8] and is reproduced in the numerical simulation. A sudden increase in flame tip velocity at x≈4 m indicates a transition to detonation in the simulation. This phenomenon was not visible as clearly in the measurements, where a more gradual increase in flame speed to 1700 m/s was detected towards the channel end. The large spacing of photodiodes for velocity measurements in this region could not resolve sharp changes in flame speed. It is not entirely clear whether DDT occurred in the experiment. Figure 6 presents pressure and numerical schlieren fields of detonation onset in the inhomogeneous mixture. The leading flame tip is initially located near the channel

top wall, and the flame is elongated due to the concentration gradient. A local explosion is observed near the leading flame tip, initiating the onset of detonation. This phenomenon is in qualitative agreement with previous experiments in unobstructed channels and mixtures with concentration gradients [2,7].

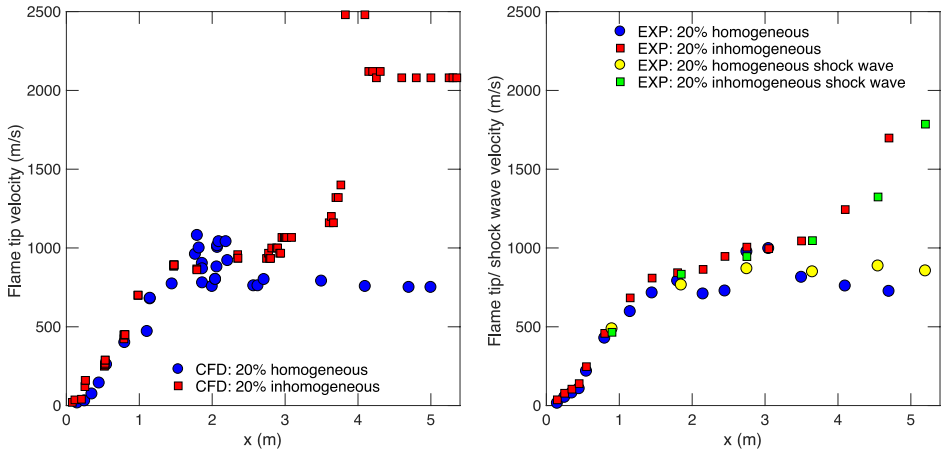

Figure 5. Comparison between flame tip velocities in homogeneous and inhomogeneous mixtures at 20% average hydrogen concentration; CFD (left) and experiments (right).

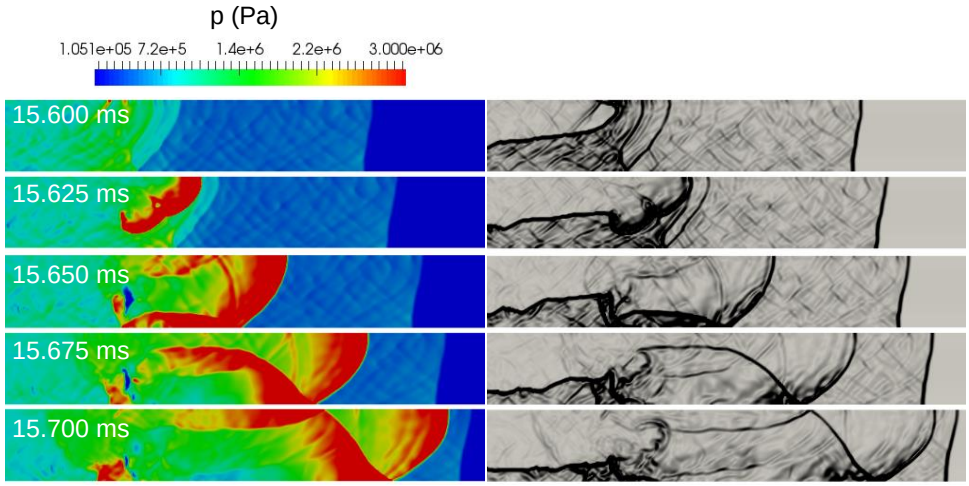

Figure 6. Pressure (left) and numerical schlieren (right) fields of detonation onset in the inhomogeneous 20% hydrogen mixture. The FOV extends from x=3.75 m to x=4.16 m**.**

6. Conclusions

Numerical studies have been conducted to investigate flame acceleration and transition to detonation in homogeneous and inhomogeneous hydrogen-air mixtures for two different average hydrogen concentrations (30% and 20% by volume) in an obstructed channel. For the numerical modelling, a density-based solver within the OpenFOAM CFD toolbox has been developed. The predictions were compared against previous experiments. Overall, the predicted flame tip velocities and locations of detonation onset are in reasonable agreement with the measurements. For both homogeneous and inhomogeneous 30% hydrogen cases, the onset of detonation occurs within the obstructed channel section. The homogeneous mixtures show slightly faster flame acceleration and earlier onset. For the 20% case, the

transition to detonation is observed only for the inhomogeneous mixture, where the concentration gradient enables stronger flame acceleration, especially in the unobstructed channel section in comparison with the homogeneous mixture. This study confirms previous findings that transverse concentration gradients in channels can lead to substantially stronger flame acceleration and a higher propensity for the transition to detonation in comparison with homogeneous mixtures at the same average hydrogen concentration.

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