Numerical Investigation of Detonation Wave Propagation through Small Orifice Holes

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Abstract

The propagation of a detonation wave in a tube filled with hydrogen-air mixture has been investigated numerically in presence of obstacles with small orifice holes. The numerical simulations are performed in a two-dimensional domain by using adaptive mesh refinement and solving inviscid compressible Euler equations for multiple thermally perfect species with reactive source term. A coarse mesh grid was used in this preliminary study, and it was observed that orifice diameters of 10, 18, 30 and 50 mm in 90 mm diameter tube initially decoupled shock wave and flame from detonation wave front. Further along the tube, the detonation wave fails to propagate in case of 10 mm diameter orifice case, however for the 18, 30 and 50 mm orifice diameter cases, the detonation wave propagated by different mechanisms of shock reflection, DDT and immediate initiation, respectively. The full paper will further analyze and validate results obtained in this preliminary study.

Keywords: Detonation, Propagation, Hydrogen-Air, Small Orifice Hole, AMROC

1 INTRODUCTION

Hydrogen has attracted wide attention as a clean fuel energy source, however safety issues associated with hydrogen have led to a lot of research being undertakes to better understand various flame propagation regimes. There are primarily two kinds of self-sustaining combustion regimes: deflagration and detonation [1]. A detonation wave differs from a deflagration wave in that the detonation wave travels at supersonic speed and pressure and temperature can have higher jump across it. Deflagration waves however travel at subsonic speeds and pressure remains almost constant and temperature increases across it. Transitions of deflagration to detonation have been studied in closed tubes [1] and it was found that obstacles in a tube can accelerate this transition [2]. However, the size of these obstacles can lead to various methods of detonation propagation through it, such as re-initiation by shock reflection, deflagration to detonation transition or even no detonation propagation[2]. In this current study, the detonation propagation is simulated in a long circular tube, which is filled with an Argon diluted hydrogen-air mixture. A single obstacle with different blockage ratios was investigated to understand the propagation mechanism of detonation waves through the orifices. An open-source program Adaptive Mesh Refinement Object-oriented C ++ (AMROC) based on Structured Adaptive Mesh Refinement (SAMR) framework [4]. This study aims to validate a numerical method with available experimental data for detonation propagation for hydrogen and develop data base for various obstacles sizes.

2 NUMERICAL METHOD

The computational domain along with initial condition used in this study are shown in Figure 1. It consists of a 1 meter long tube with an orifice plate, located 200 mm from left wall, used as the obstacle. The orifice plate has a thickness of 10 mm with orifice plate hole diameter varied between s = 10, 18, 30 and 50 mm. The tube is filled with a H_2:O_2:Ar mixture with a ratio of 2:1:7 at a pressure of 10 kPa and a temperature 298 K. Slip and adiabatic boundary condition are assumed at the wall and the tube outlet is considered as a supersonic outlet boundary. A regular oscillating detonation wave propagation with a C-J speed of 1638.5 m/s has been imposed up to 10 mm distance from left end of tuve at time, t =0. The temperature, pressure and OH mass fraction plots for developed detonation front before the obstacle has been shown in Fig. 1b. In this preliminary study, the initial grid size is considered as 1 mm $\times$ 1 mm, and 3 level of refinement was used. The gradient of pressure, temperature and density have been used to control the adaptive mesh refinement and coarsening. The unsteady computation has been performed up to 800 μs with an auto-adjusted time step based on an effective CFL number of 0.95.

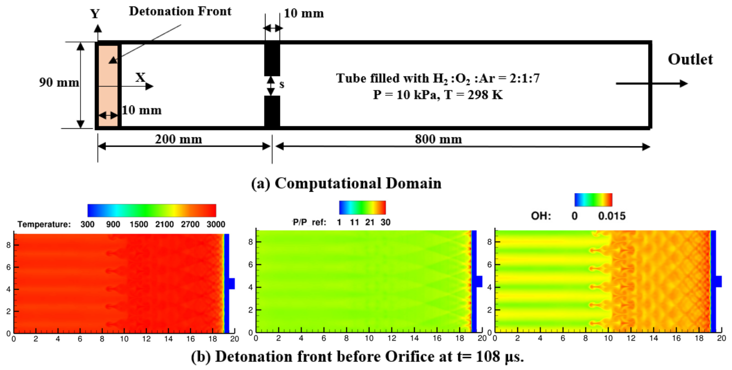

Figure 1: (a) Computational Domain (b) Detonation front after 108 μs of initialization

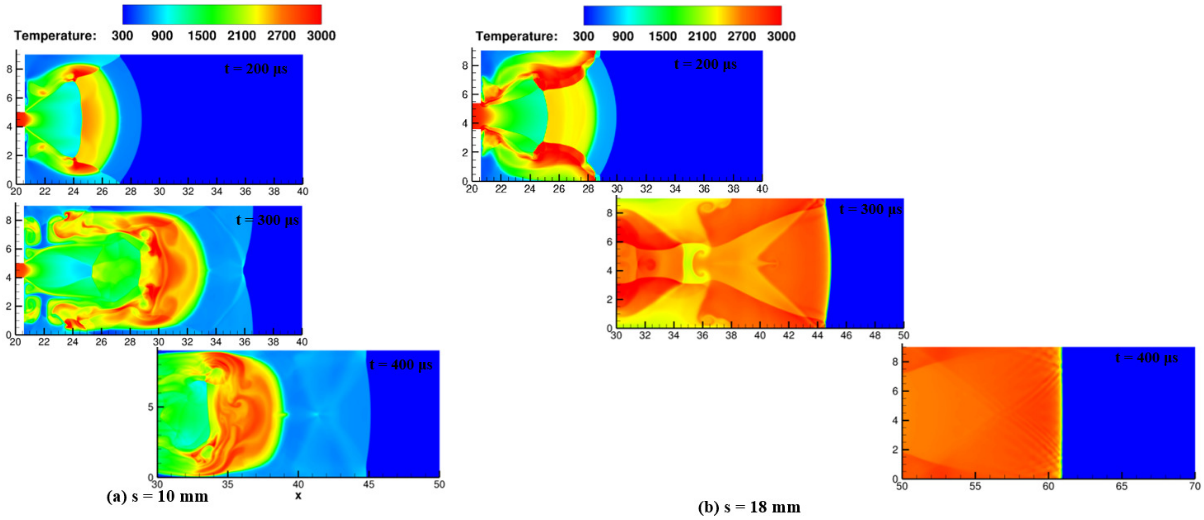

Figure 2: Detonation Wave Propagation for orifice diameter (a) 10 mm (b) 18 mm

3 PRELIMINARY RESULTS

Figure 2 and 3 show preliminary simulation results for the temperature contour plots. These temperatures are plotted at three distinct time instances t = 200, t = 300 and t = 400 μs. Based on the location of the flame front a window snapshot of 20 mm was taken and placed at a relative distance to the previous time plot. Fig. 2a shows propagation of a detonation wave through a 10 mm orifice hole diameter. At t = 200 μs, it can be seen that the flame and shock wave have decoupled completely. At t= 300 and t = 400 μs, the shock moves ahead of the flame (high temperature zone) and overall the detonation wave fails to propagate as a detonation wave and turns into a moving deflagration wave. Figure 1b shows temperature contours of a detonation wave propagation through an orifice with an 18 mm hole diameterm. Initially at t = 200 μs, the shock and flame remain decoupled. But, at t = 300 and t = 400 μs temperature contours show DDT transition and propagation of the detonation wave. Similarly, Fig 3a and 3b show detonation wave propagation through orifice holes of diameter 30 mm and 50 mm. The propagation through the 30 mm hole shows decoupling and later detonation wave transition through shock reflection. However, detonation wave propagation through a 50 mm diameter orifice shows instantaneous detonation propagation. The full paper will include discussions of flow features and propagation mechanisms through these hole sizes with validated results.

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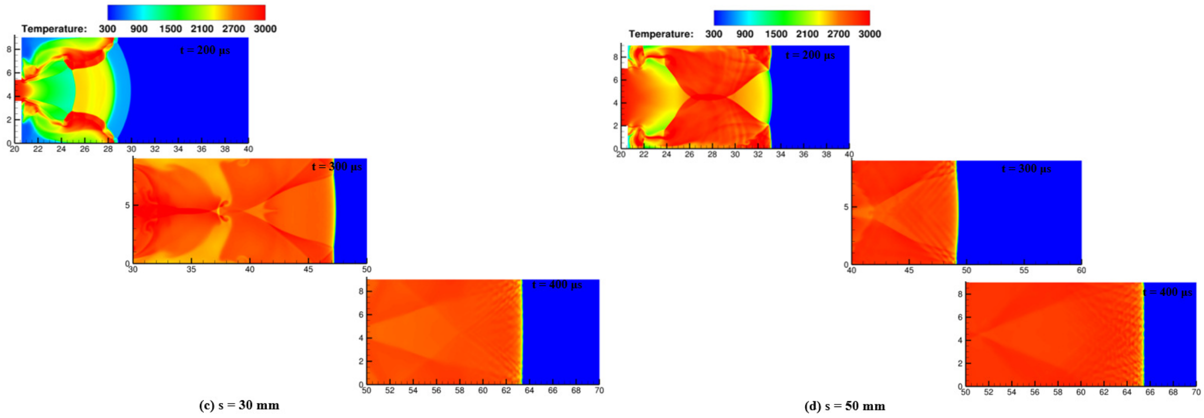

Figure 3: Detonation Wave Propagation for orifice diameter (a) 30 mm (b) 50 mm

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