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# Adaptive simulations of cavity-based detonation in supersonic hydrogen—oxygen mixture



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#### ABSTRACT

Two-dimensional reactive Euler equations with a detailed reaction model where the molar ratio of the combustible mixture H<sub>2</sub>/O<sub>2</sub>/Ar is 2:1:7 under the condition of pressure 6.67 kPa and temperature 298 K, are solved numerically with adaptive mesh refinement method to investigate detonation combustion using a hot jet initiation in cavity-based channels filled with the supersonic combustible mixture. Results show that from the comparison between the simulations in a cavity-based channel and a straight channel without any cavity embedded, it is indicated that the cavity can help realize detonation initiation in the combustible mixture with a hot jet. It is suggested that detonation initiation can be realized using a relatively weaker hot jet in cavity-based channels filled with the supersonic combustible mixture compared with that in straight channels without a cavity embedded. The cavity also plays a significant role in detonation propagation in the supersonic combustible mixture. After the hot jet is shut down, the acoustic wave generated by the subsonic combustion in the cavity can accelerate detonation propagation through a subsonic channel and result in the formation of a slightly overdriven detonation eventually. For a given flow with a shadow cavity embedded, there should exist a minimum cavity width  $L_{min}$ . When the width is below  $L_{min}$ , only some pressure oscillations in the cavity can make some impacts on detonation initiation and propagation. Otherwise, cavity oscillations can be generated which can greatly accelerate detonation initiation and propagation in the supersonic combustible mixture. For the shadow cavity, purely increasing the cavity depth does not have any more influence on detonation combustion. However, if the cavity is a deep one, it can play an important role in accelerating detonation initiation and propagation in the supersonic combustible mixture due to resonant oscillations.

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#### Introduction

Detonation combustion is an extremely effective method which can burn combustible mixtures and release chemical energy efficiently. The idealized thermodynamic efficiencies

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of constant pressure, constant volume, and detonation are 27%, 47%, and 49%, respectively [1]. Due to the inherent theoretical advantage of detonation over deflagration, investigations on detonation based engines have been promoted significantly [2–4].

The development of reliable initiation method is always one of the most important issues for detonation combustion. Direct initiation [5–7] can ignite detonation quickly, but it is not actually applicable due to its necessary usage of large energy. An alternative approach is the utilization of a hot jet which can also ignite detonation very fast [8], because the flame acceleration process of deflagration to detonation transition (DDT) is bypassed essentially. The hot jet initiation has been investigated comprehensively in quiescent combustible mixtures [9-12], but in supersonic combustible mixtures only a few experimental researches have been carried out [13-15]. Ishii et al. [13] conducted experiments in combustible mixtures whose Mach numbers were 0.9 and 1.2 to investigate detonations using a hot jet initiation. Han et al. [14,15] studied detonation initiation and DDT process using a hot jet experimentally in supersonic hydrogen-air mixtures with Mach numbers 3 and 4, where detonations were initiated through shocks or shock reflections [16-20] on the walls induced by the hot jet. A series of simulations on detonation combustion in straight channels with a hot jet initiation in supersonic hydrogen-oxygen mixtures were conducted by Cai et al. [21-25] and Liang et al. [26], where the SAMR (Structured Adaptive Mesh Refinement) framework [27] based open-source program AMROC [28-32] (Adaptive Mesh Refinement Object-oriented C++) is utilized. These numerical simulations solved the two-dimensional and threedimensional reactive Euler equations and applied a classical second-order accurate MUSCL-TVD (Monotone Upstreamcentered Schemes for Conservation Laws-Total Variation Diminishing) scheme with both a simplified reaction model [29] and a detailed reaction model [33]. It was shown by these results that for a given hot jet and flow condition there exists a critical hot jet width below which detonation initiation cannot be realized and when the hot jet is shut down no other methods can be utilized for the control of detonation propagation. It is indicated that it is difficult to realize detonation initiation purely using a hot jet and stabilization control of detonation propagation in straight channels. Therefore, some other approaches might be needed to be cooperated together for a better configuration.

Currently, cavities are widely investigated on the feedback mechanism [34–36], especially they have been successfully used as flameholders in supersonic combustors due to their outstanding potential to stabilize combustion by cavity oscillations [37–39]. However, they have not been tried so far associated with detonation combustion in supersonic combustible mixtures. To investigate the potential usage of cavities on detonation initiation and propagation, high-resolution simulations are conducted in cavity-based channels filled with supersonic combustible mixtures using the adaptive mesh refinement method.

The remainder of this paper is organized as follows: the computational setup is presented in Section 2, including the introduction of the computational model and numerical scheme. A convergence analysis is discussed in Section 3.

Results of the simulations are shown in Section 4, in which cavity-based detonation initiation and propagation, and effects of different cavity sizes including the width and depth, are investigated. Finally Section 5 concludes the paper.

#### **Computational model**

#### **Computational setup**

The simplified schematic for the calculation model is depicted in Fig. 1. Reflecting boundaries with slip wall conditions are used on the upper and lower wall. A small inflow which models a hot jet, is embedded into the lower wall boundary. A cavity is located downstream in the hot jet. Numerical simulations and experimental observations [40-43] indicate the existence of two types of detonation structures which are usually classified as regular (weakly unstable) and irregular (highly unstable) detonations based on the regularity of cellular structure [44-51]. Self-sustaining CJ (Chapman-Jouguet) detonations for hydrogen-oxygen mixtures highly diluted with argon in low pressure are ideal candidates for detonation simulations, because very regular cellular detonations can be generated [52], which are relatively beneficial for investigations of cavity-based detonations. The cavitybased channel consists of a stoichiometric H<sub>2</sub>/O<sub>2</sub>/Ar mixture with a molar ratio 2:1:7 under the condition of pressure 6.67 kPa and temperature 298 K. The mixture is flowing in the channel at the CJ velocity (the referenced  $V_{CJ} = 1627$  m/s). The right boundary models the inflow condition and the ideal outflow condition is imposed on the left one.

The hot jet is set to the equilibrium CJ state of  $H_2/O_2$  with a stoichiometric molar ratio under the condition of pressure 6.67 kPa and temperature 298 K. This equilibrium CJ state is calculated with Cantera [53], as shown in Table 1.

#### Numerical scheme

The two-dimensional reactive compressible flow utilizes the Euler equations with the detailed reaction model [33] as governing equations. The second-order accurate MUSCL (Monotone Upstream-centered Schemes for Conservation Laws)-TVD finite volume method (FVM) is used for the convective flux discretization. The hydrodynamic solution is separated into the flux calculation step and reconstruction step. Rather than Strang splitting, Godunov splitting is adopted here due to almost the same performance with Strang splitting but more



Fig. 1 – The schematic of the calculation model.

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