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Detonation Interaction with Cavity in Supersonic Combustible Mixture

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1 **Nomenclature**

2 D = depth of the cavity, cm
L = width of the cavity, cm
l_{ig} = induction length of one-dimensional Zel'dovich–von Neumann–Döring model, mm
Pts/l_{ig} = number of the grid points distributed in the induction length
V_{CJ} = Chapman–Jouguet velocity, m/s
X_1 = length of the straight channel, cm
X_2 = width of the hot jet, cm
X_3 = distance from the hot jet edge to the front edge of the cavity, cm
X_4 = distance from the rear edge of the cavity to the outflow
3 boundary, cm
Y_1 = height of the channel, cm

I. Introduction

DETONATION has a higher thermodynamic efficiency than deflagration [1,2]. Detailed understanding of detonation combustion is important not only for accessing the threat from accidental explosion but also for innovative propulsion applications [3,4]. Although detonation has been widely studied as an ongoing research for several decades, most investigations are carried out in quiescent or low-speed gases. Different from those in quiescent gases, understanding the behavior of detonation combustion in supersonic combustible mixtures is important for detonation physics and practical applications.

Based on the preceding idea, a series of numerical simulations [5–9] on detonation combustion in supersonic combustible mixtures have been performed, where the open-source program Adaptive
Mesh Refinement in Object-Oriented C++ (AMROC) [10–14] based 4
on the structured adaptive mesh refinement framework [15,16] is adopted to solve the reactive Euler equations with the robust second-order-accurate monotone upstream-centered schemes for conservation laws (MUSCL)–total variation diminishing (TVD) scheme. Initially based on the Distributive Adaptive Grid Hierarchies software, AMROC currently supports several Euler solvers for gas mixtures with a complex equation of state based on TVD and weighted essentially nonoscillatory schemes and is integrated in the Virtual Test Facility software. Although a hot jet is used, detonation initiation is actually realized resulting from shock reflections or Mach reflections [17–20] induced by the hot jet. These numerical simulations are carried out in simplified straight channels, mainly concentrating on detonation initiation and its propagation characteristics in supersonic combustible mixtures.

Because of the outstanding potential to stabilize combustion by cavity oscillations [21–27], recently detonation combustion has been numerically investigated in cavity-based channels filled with a supersonic hydrogen–oxygen mixture [28]. It is reported that the cavity can help realize detonation initiation and accelerate its propagation in the supersonic combustible mixture due to pressure wave enhancement resulting from subsonic combustion in the cavity. However, the initiated detonation always maintains upstream in the cavity because of limitation of the incoming flow velocity. In practice, the incoming velocity may vary when the flight is accelerating. When the incoming velocity is larger than the Chapman–Jouguet (CJ) velocity, the detonation may propagate downstream and further interact with the cavity, and whether it can lead to detonation failure or not in a cavity embedded channel is still unknown. Therefore, it is necessary to clarify the potential influence of detonation interaction with the cavity on detonation propagation and its sustainment. Following the previous study, AMROC is employed for high-resolution numerical simulations using a detailed reaction model [29] to investigate detonation wave interaction with cavity and further its influence on detonation evolution in supersonic combustible mixtures. The hydrogen–oxygen reaction mechanism consists of 34 elementary reactions and considers nine species (H, O, OH, H_2, O_2, H_2O, HO_2, H_2O_2, and Ar). It is originally extracted from the larger hydrocarbon mechanism and has been validated for hydrogen detonations [10–13]. This work is part of an ongoing research program, aiming at providing information to help improve the overall understanding of detonation combustion in supersonic combustible mixtures.

The remainder of this paper is organized as follows. The computational model is presented in Sec. II, including the introduction of the computational setup and numerical scheme. A convergence analysis is discussed in Sec. III. Results and analysis are shown in Sec. IV, in which detonation interaction with the cavity and effects of channel height are investigated. Finally, Sec. V concludes the paper.

II. Computational Model

A. Computational Setup

Figure 1 shows the schematic of the calculation model. A small inflow is embedded into the lower wall, which is used to model a hot jet injection. A cavity is located downstream in the hot jet. Reflecting boundaries with slip wall conditions are adopted on the upper and lower walls. Because of generation of regular cellular patterns, self-

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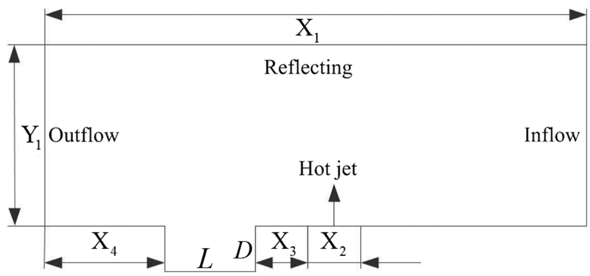

Fig. 1 Schematic of the calculation model.

sustaining CJ detonations for hydrogen–oxygen mixtures highly diluted with argon in low pressure are ideal candidates for detonation simulations [30]. Here, a stoichiometric $H_2/O_2/Ar$ mixture with a molar ratio $2:1:7$ under the condition of pressure 6.67 kPa and temperature 298 K is used, which has been extensively demonstrated to produce very regular cellular detonation [31,32]. The mixture flows in the channel at a given velocity. 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 a H_2/O_2 mixture with a stoichiometric molar ratio under the condition of pressure 6.67 kPa and temperature 298 K [28]. To model the sonic injection in experiments, the injection velocity of the jet is set to the local sonic speed to make it a chocked one. This equilibrium CJ state is calculated with Cantera [33], as shown in Table 1. When dealing with the boundary condition for the hot jet, the parameter "time" is considered to control the injection duration. When the hot jet is shut down, the inflow condition of the hot jet will be switched to reflecting condition immediately.

B. Numerical Scheme

The two-dimensional reactive Euler equations with the detailed reaction model are used as the governing equations. The second-order-accurate MUSCL-TVD finite volume method 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
5 having to almost the same performance with Strang splitting but being more computationally efficient [10]. A hybrid Roe–HLL [10] Riemann solver is used for the construction of the inter-cell numerical upwind fluxes, whereas the Van Albada limiter is applied with the MUSCL reconstruction to construct a second-order method in space. As for time integration, the second-order-accurate MUSCL–Hancock technique [34] is adopted. Under the condition of Courant–Friedrichs–Lewy number 0.95, the dynamic time step is used for all the simulations.

Table 1 Equilibrium CJ state for the hot jet[a]

State parameter	Value
Pressure	113,585.12 Pa
Temperature	3,204.8374 K
Density	0.05959 kg/m^3
Velocity	1,229.9015 m/s
Energy	83,445.813 J/m^3
H_2	0.024258141648492
H	0.007952664033931
O	0.055139351559790
O_2	0.124622185271180
OH	0.161144120322560
H_2O	0.626759466258162
HO_2	0.000117215557650
H_2O_2	0.000006855348235
Ar	0

[a]The parameters for the nine species are given by the mass fractions.

For the shock-capturing method used in the simulations, the introduced numerical diffusion is determined by grid resolution [35]. At low grid resolution, numerical diffusion dominates over physical diffusion, whereas at high grid resolution, physical diffusion dominates over numerical diffusion. Because of low numerical diffusion and absence of physical diffusion in high-resolution simulations solving the Euler equations, small-scale unphysical features can be generated, yet it is found that, even in high-resolution detonation simulations, the Euler and Navier–Stokes solutions are qualitatively similar [36]. It is reported that, although the diffusion effect plays an influential role in the evolution of irregular detonations [37,38], it does not contribute significantly to regular detonations due the absence of hydrodynamic instabilities involved with regular detonations (i.e., the Kelvin–Helmholtz instability and Richtmyer–Meshkov instability) [39,40]. Therefore, the results obtained in the present work where the reactive Euler equations are used for regular detonations are nevertheless expected to give at least qualitatively correct conclusions.

III. Verification of Adaptive Mesh Refinement

As shown in Fig. 1, $X_1 = 10$ cm, $X_2 = 0.3$ cm, $X_3 = 0.4$ cm, $X_4 = 3$ cm, and $Y_1 = 3$ cm with the initial mesh 400×160. The cell size of the CJ detonation under the given condition is $\lambda = 3.0$ cm, and so one whole detonation cell can be generated in the Y direction for this setup. The width and depth of the cavity are $L = 2$ cm and $D = 1$ cm, respectively. Based on previous experiments [41], a division between shallow and deep cavities is $L/D \cong 1$. When $L/D > 1$, the cavities can be considered shallow, whereas when $L/D < 1$, the cavities are considered deep. Therefore, the cavity used in the present work is considered as a shallow one. The induction length of one-dimensional Zel'dovich–von Neumann–Döring (ZND) model under the condition is $l_{ig} = 1.509$ mm, which is calculated using Cantera. The characteristic time as the channel height by the CJ velocity (Y_1/V_{CJ}) is used for dimensionless time in the following results.

For the detailed reaction model used here, a minimal 6 Pts/l_{ig} spatial resolution has been suggested for the ZND solution to resolve accurately all the intermediate reaction products [42]. However, in multidimensional detonations, a higher resolution is required for complete capture of internal wave structures around triple points. An effective resolution of up to 44.8 Pts/l_{ig} is used in two-dimensional verification simulations of regularly oscillating detonations, which indicate that this resolution is sufficient for resolving reliably even the secondary triple points [10]. This grid resolution has also been demonstrated to obtain at least qualitatively correct results for multidimensional detonation simulations with the detailed reaction model in previous investigations [31,32].

Here, a three-level refinement with refinement factors $r_1 = 2, r_2 = 4$ is adopted for all the following simulations, which eventually gives a highest grid resolution of 48.3 Pts/l_{ig}. In the present work, the detonation wave interaction with the cavity is mainly focused on, and it is believed that this grid resolution can satisfy the requirement for resolving the main features.

IV. Results and Analysis

The detailed process of detonation initiation using a hot jet in a cavity-embedded channel has been illustrated previously in detail [28], where the velocity of the supersonic incoming flow is given as the corresponding V_{CJ}. To have a quick understanding of this issue, a very brief introduction is provided here. After the injection of a hot jet into the supersonic flow, a bow shock is first induced and further reflects on the upper wall when it becomes adequately strong. Because of the continuous strength enhancement of the bow shock, a Mach reflection is eventually formed on the upper wall, which has been demonstrated to be actually a local Mach detonation (Mach stem-induced detonation) [6]. The Mach detonation continues forward propagation and eventually results in a second reflection on the lower wall. The Mach detonation reflection, which serves as a strong ignition source, contributes significantly to the realization of a complete detonation initiation in the whole channel.

In the previous work [28], when the incoming velocity is given as the CJ velocity, the detonation front is almost sustained at the same location upstream in the cavity after the hot jet is shut down due to cavity oscillation. It is suggested that, for a successful detonation wave interaction with cavity, the incoming flow velocity should be higher than the corresponding CJ velocity to ensure downstream propagation of detonation after the hot jet shutdown. However, if the incoming velocity is large enough, detonation initiation might not be realized successfully when the hot jet remains the same [4]. Therefore, here the velocity of the supersonic incoming flow is given a value of $V = 1.05V_{\mathrm{CJ}}$. It is slightly higher than the CJ velocity, which can confirm both successful detonation initiation and its interaction with the cavity.

A. Detonation Attenuation and Interaction with the Cavity

Because of the contractive passway mechanism induced by hot jet [43], overdriven detonation is generated after initiation as it propagates forward toward the supersonic combustible mixture with the CJ velocity. After the shutdown of the hot jet, detonation cannot remain the same overdriven state but gradually attenuates, as shown in Fig. 2.

In Fig. 2a, immediately after the shutdown of the hot jet, an expansion wave is observed. At this moment, five triple points are generated; however, for a CJ detonation under the given condition, normally only two triple points are formed in the channel [43], indicating the formation of an overdriven detonation here. Because of the intrinsic inertia, the detonation continues to propagate forward for a while until it reaches the farthest propagation location approximately at $X = 7.3$ cm, as shown in Fig. 2b, where the influence of the hot jet on the detonation front can be recognized as totally dissipated. Subsequently, the detonation begins its backward propagation, continuously undergoing the attenuation process associated with the decreasing of propagation speed and strength of the detonation front. As a result, as shown in Fig. 2c, detonation attenuation results in a reduction of numbers of both transverse waves and triple points [43]. Compared with that in Fig. 2b, only three triple points can be observed on the detonation front in Fig. 2c due to the further attenuation.

Figure 3 illustrates the process when the detonation wave crosses over the cavity. As shown in Fig. 3a, an oblique shock wave is generated within the detonation front and separated from the reaction front following behind, which is a typical structure of detonation bifurcation. Also, an unburned jet is generated associated with the oblique shock, as shown in Fig. 3b. The unburned jet is gradually consumed through the diffusion effect with burned gases [39]. It should be noted that, because of the absence of physical viscosity in the adopted Euler equations, only the numerical dissipation contributes to the diffusion effect. As shown in Fig. 3c, the unburned jet becomes much larger as the oblique shock wave continues growing. The detonation wave, which is shortened ulteriorly compared with that in Fig. 3b, further propagates backward, even speculating that the detonation may fail and disappear eventually.

B. Detonation Sustainment and Forward Propagation

However, rather than failure or disappearance, the detonation wave realizes dynamical sustainment at approximately $X = 3.5$ cm for a while during the backward propagation, as shown in Fig. 4. Within the three successive frames, the oblique shock wave is gradually lifted up with the angles of 36.07, 40.27, and 45.43 deg, respectively.

It is reported that a low-speed recirculation region can be created in a cavity in supersonic combustion, and partial subsonic combustion within the recirculation flow acts as a continuous ignition source for the whole flow, thus eventually achieving flameholding in supersonic incoming flows [23–25]. Because of pressure oscillations resulting from the subsonic combustion, as shown in Fig. 5, the shear layers behind the oblique shock wave become highly unstable and even turbulent associated with the generation of plenty of vortices mainly due to the Kelvin–Helmholtz (KH) instability. Therefore, the consumption of the unburned jet behind the oblique shock wave is enhanced through the rapid mixing effect. Hence, the further

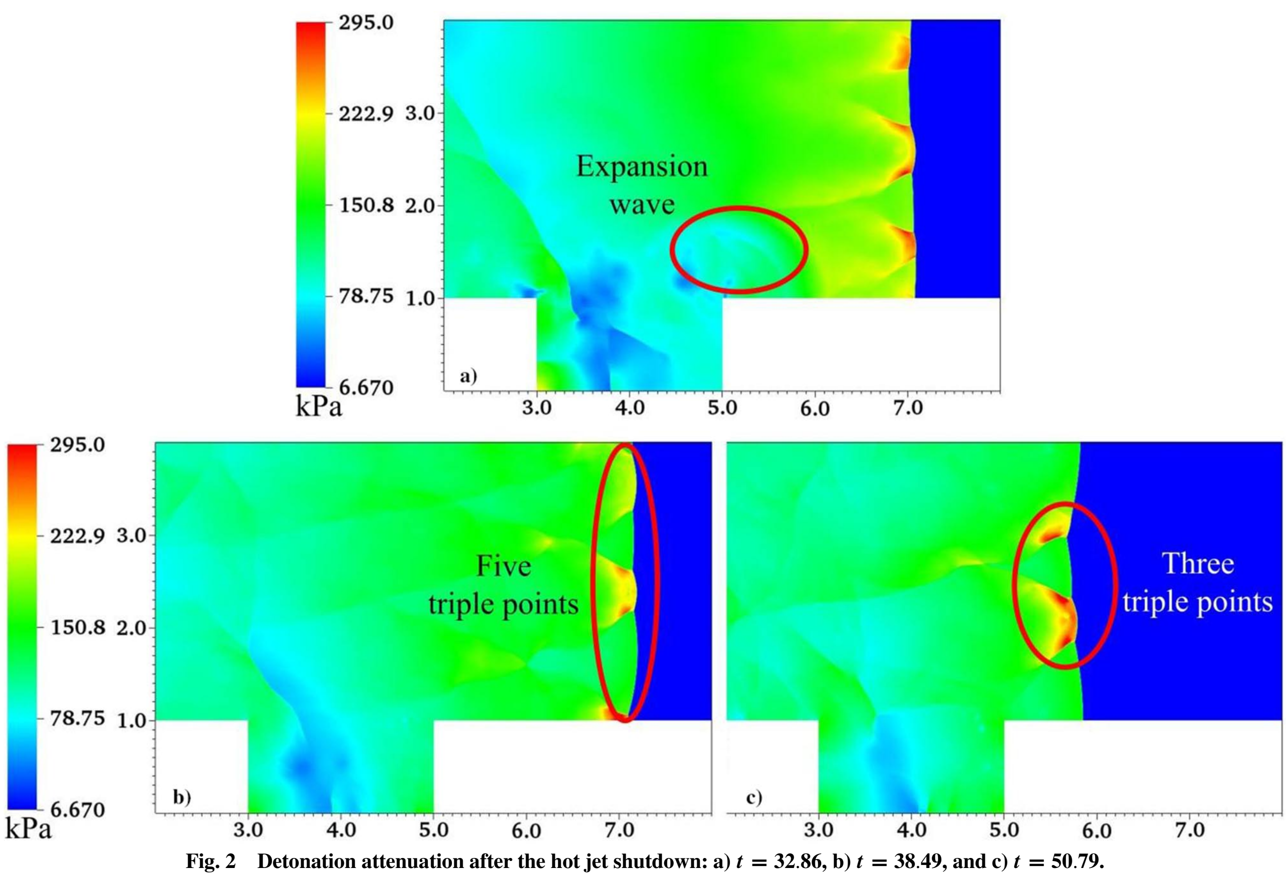

Fig. 2 Detonation attenuation after the hot jet shutdown: a) $t = 32.86$, b) $t = 38.49$, and c) $t = 50.79$.

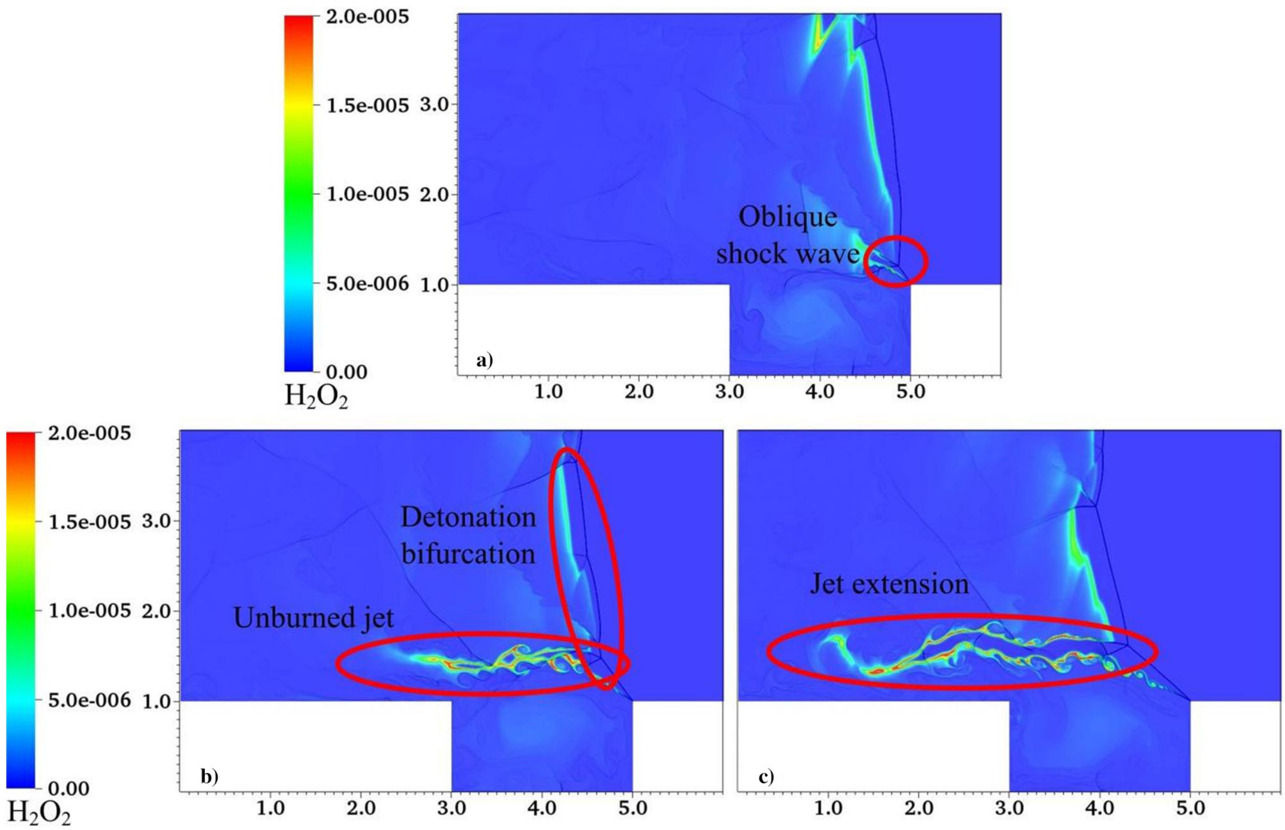

Fig. 3 Detonation evolution when crossing through the cavity: a) $t = 56.84$, b) $t = 60$, and c) $t = 63.17$.

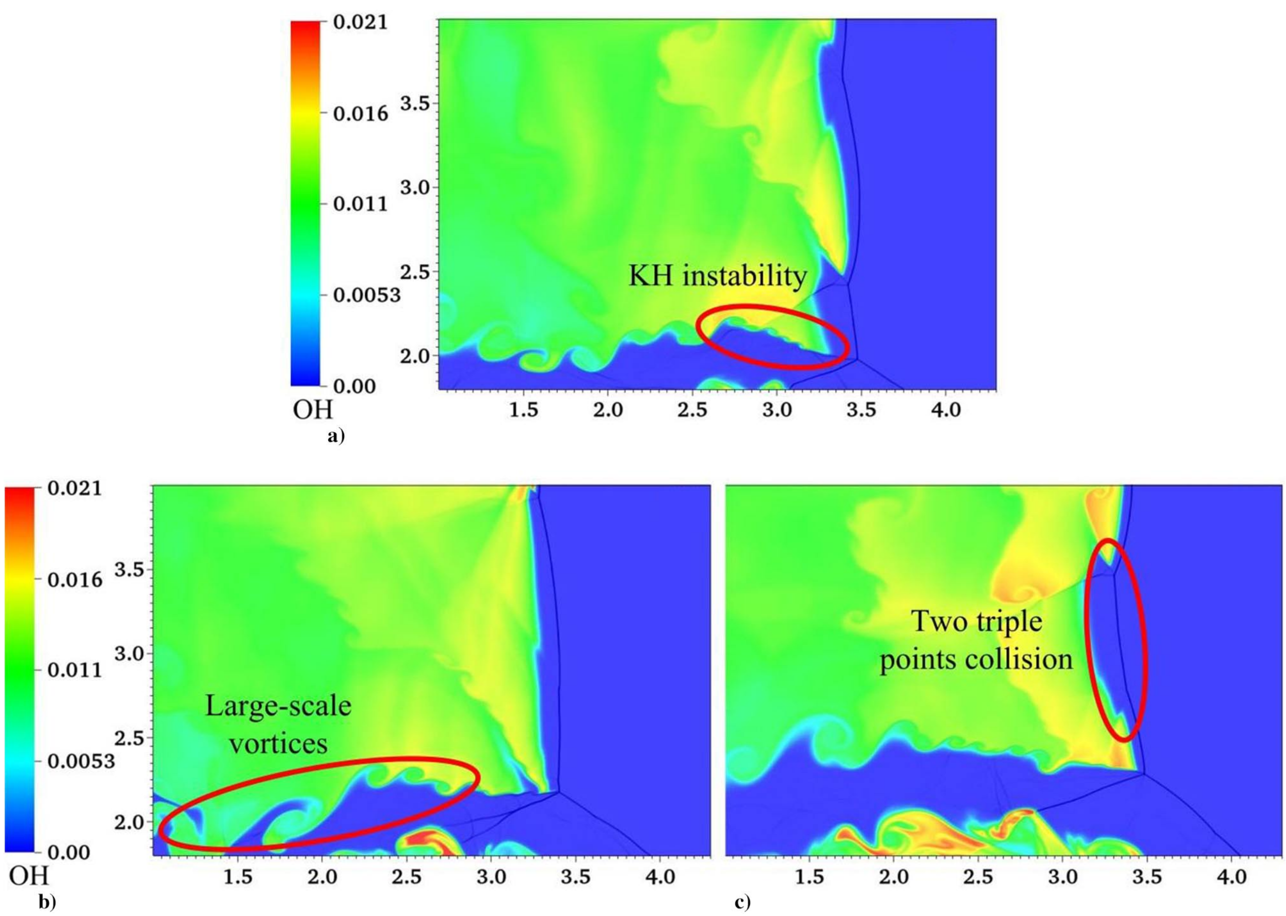

Fig. 4 Detonation sustainment over the cavity: a) $t = 67.60$, b) $t = 68.97$, and c) $t = 70.35$.

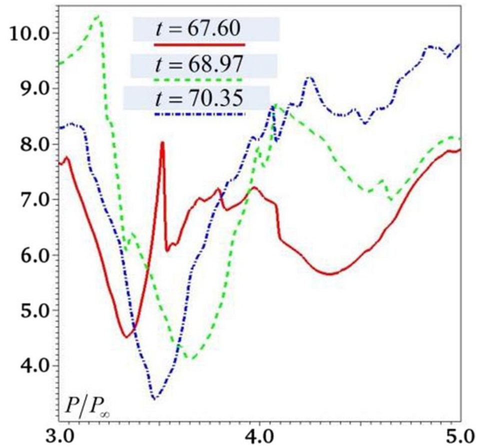

Fig. 5 Pressure oscillations at $Y = 0.5$ cm within the cavity.

increased heat release leads to an increase of temperature and pressure in the cavity, which further benefits lifting up of the oblique shock wave and dynamical sustainment of detonation.

As the oblique shock wave lifts up, the shear layers undergo an obvious transformation. Because of hydrodynamic instabilities, large-scale vortices are generated along the highly unstable shear layers, which can accelerate the rapid mixing and subsequent chemical heat release, further facilitating the lifting up of the highly unstable shear layers. Compared with the head of the shear layers, the tail of the shear layers is raised more quickly, thus resulting in formation of a contractive passway together with the upper wall when the shear layers are considered as free boundaries.

It is reported that contractive passway can prevent the expansion of detonation products effectively, thus resulting in forward propagation of detonation and eventually formation of overdriven detonation [43]. After the collision of the two triple points in Fig. 4c, which can instantaneously realize intense heat release, forward propagation of detonation occurs once again, as shown in Fig. 6. This is different from that previously discussed with the continuous injection of the hot jet. The unburned jet behind the oblique shock wave is highly precompressed, hence being consumed quickly and resulting in realization of overdriven detonation immediately in the whole channel once again.

C. Periodical Propagation

Although forward propagation of detonation is achieved again, it cannot be sustained without continuous injection of hot jet [3]. After overdriven detonation reaches the farthest location when propagating forward, it will begin to attenuate and establish its backward propagation again. Hence, because of detonation interaction with the cavity, forward propagation, detonation attenuation, and detonation sustainment are completed in the channel, which together make up a periodical process. It is indicated that dynamical sustainment propagation of detonation can be realized in supersonic combustible mixtures when the incoming velocity is higher than the CJ velocity in cavity-based channels.

It should be noted that if no cavity is embedded in the channel, the attenuated detonation will finally fail and disappear in the channel [43]. Based on this comparison, it is suggested that the cavity-based setup plays an important role in the relatively dynamical sustainment propagation of detonation in supersonic combustible mixtures.

D. Effects of Channel Height

When the detonation wave crosses through the cavity, detonation bifurcation is generated, which is highly dependent on the channel height [44]. The structure of detonation bifurcation exists in the whole periodical process, hence being very important for detonation wave interaction with the cavity. Therefore, a series of simulations are

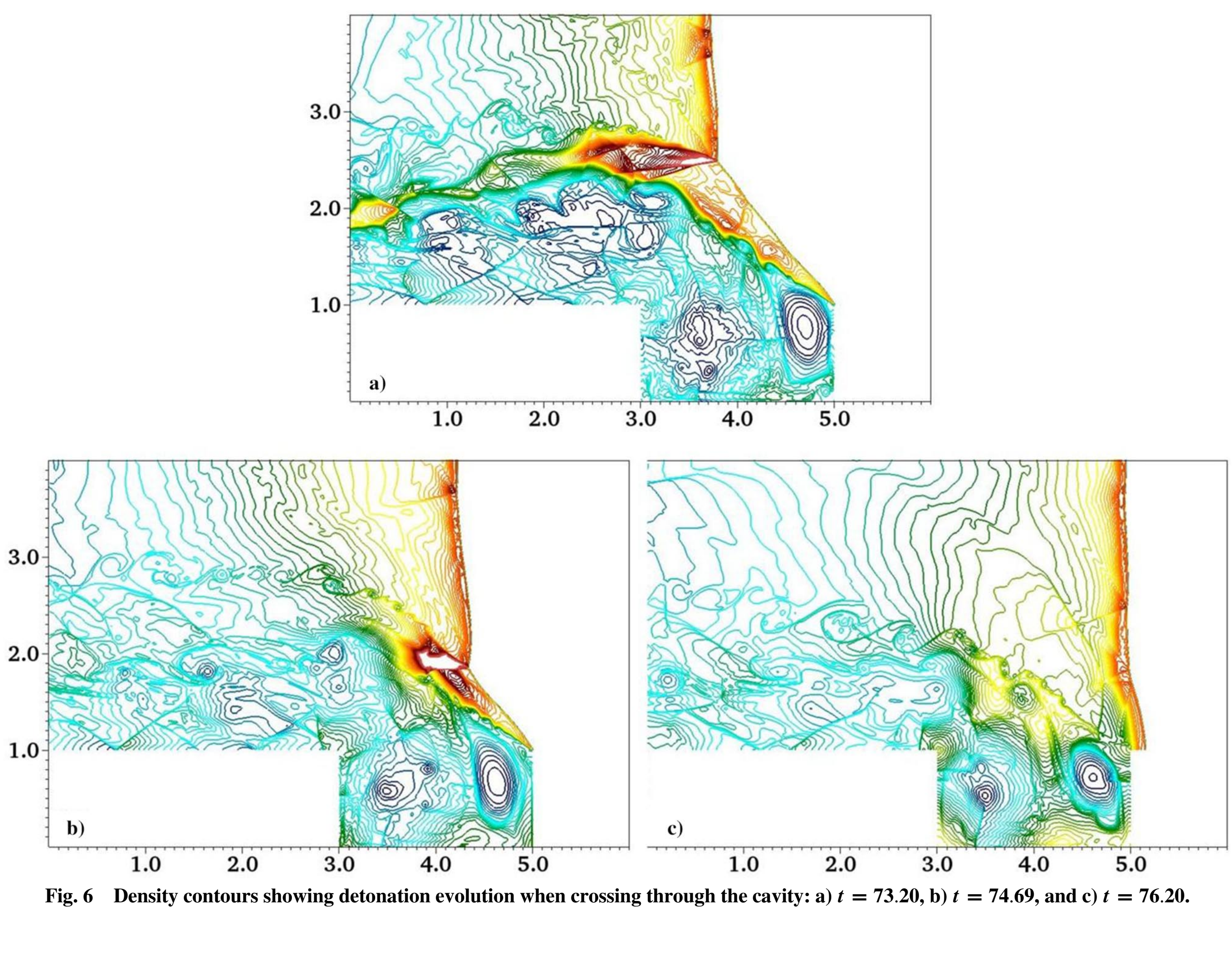

Fig. 6 Density contours showing detonation evolution when crossing through the cavity: a) $t = 73.20$, b) $t = 74.69$, and c) $t = 76.20$.

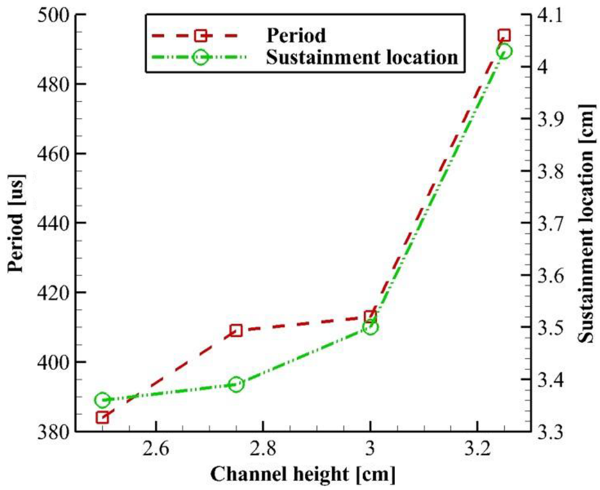

Fig. 7 Periods and sustainment locations for different channel heights.

conducted to provide an elementary understanding of channel height effects on detonation wave interaction with the cavity associated with detonation bifurcation in supersonic combustible mixtures. The effects of channel height are investigated independently while the other parameters are all kept the same.

Based on the preceding case, five different channels with heights varied from $Y_1 = 2.5$ cm to $Y_1 = 3.5$ cm ($Y_1 = 2.5, 2.75, 3.0, 3.25$, and 3.5 cm) are investigated. For the cases when $Y_1 = 2.5, 2.75, 3.0$, and 3.25 cm, forward propagation is all realized once again after undergoing detonation wave interaction with the cavity, which takes a gradually longer period for the whole periodical process with the increasing of the channel height, especially for the case when $Y_1 = 3.25$ cm, as shown in Fig. 7. In addition, sustainment location also increases with the channel height, indicating that the size of detonation bifurcation reduces with the increasing of channel height. When $Y_1 = 3.5$ cm, detonation initiation is not realized successfully due to the absence of Mach reflection on the upper wall [3]. For this case, utilization of a stronger hot jet is necessary for successful initiation.

When the channel height is small, detonation bifurcation resulting from detonation wave interaction with the cavity occupies a large part of the whole channel, thus contributing significantly to forward propagation of detonation once again. However, when the channel height is large, the detonation front plays a dominant role in the periodical process. For this case, detonation wave interaction with the cavity has only limited influence on preventing detonation attenuation. Therefore, it is speculated that when the channel height increases further, detonation wave might not propagate forward once again but realize dynamical sustainment over the cavity due to detonation wave interaction with cavity or finally fail when the channel height is large enough.

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V. Conclusions

Two-dimensional detonation simulations are carried out in cavity-based channels to investigate detonation wave interaction with cavity in supersonic combustible mixtures. The results are as follows.

1) When the detonation wave crosses over the cavity during backward propagation, an oblique shock wave is first originated from the left edge of the cavity, resulting in the formation of detonation bifurcation associated with an unburned jet.

2) Rather than failure and disappearance, the detonation wave realizes relatively dynamic sustainment during backward propagation. Large-scale vortices along the highly unstable shear layers due to the KH instability enhance the mixing effect, accelerate the consumption of the unburned jet, and further the subsequent chemical heat release, which plays a significant role in detonation sustainment.

3) A periodical process of forward propagation, detonation attenuation, and detonation sustainment is formed due to detonation wave interaction with cavity, thus being able to avoid detonation failure in cavity-based channels when the incoming velocity is higher than the CJ velocity.

4) When increasing the channel height, forward propagation is realized once again after undergoing detonation wave interaction with the cavity but takes a longer period. However, the detonation wave might realize dynamical sustainment over the cavity or finally fail when the channel height is large enough.

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