



Dynamical Detonation Propagation in Supersonic Expanding Combustor

Embedded with a Cavity

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Abstract

In the present work dynamically quasi-steady propagation of detonation is investigated in supersonic expanding channels with a cavity embedded. The two-dimensional reactive NS equations and one-step two-species reaction model are solved using a hybrid high-order WENO-CD scheme associated with structured adaptive mesh refinement. The results show that after the shutdown of the hot jet, dynamically quasi-steady propagation of detonation can be realized in the supersonic expanding channel with the cavity during the backward propagation with an overall configuration of detonation bifurcation. In the supersonic expanding channel with the cavity, quasi-steady propagation of detonation is realized mainly due to the two different effects: the one that can facilitate detonation propagation resulting from pressure oscillations in the cavity and the other that can lead to detonation attenuation because of the Prandtl-Meyer expansion fan resulting from the expanding wall, respectively. When the incoming velocity is lower than the CJ one, dynamic stabilization of detonation still cannot be achieved, suggesting that supplementary methods should be utilized for the dynamically quasi-steady propagation of detonation under this circumstance; however, when the incoming velocity is larger than the CJ one, dynamically quasi-steady propagation of detonation can be realized effectively due to the formation of a periodic process of backward propagation, detonation bifurcation and forward propagation, indicating the importance of the expanding channel with the cavity on dynamical stabilization of detonation in supersonic flows for incoming velocity larger than the CJ one.

Keywords: *Supersonic combustible mixture; Expanding channel with cavity; Dynamically stationary propagation of detonation; Stabilization mechanism*

1. Introduction

Due to the superior performance at high Mach numbers ($Ma \geq 5.0$), scramjets have become one of the first choices for hypersonic air-breathing propulsion systems. It is believed that the performance of the scramjet might be improved significantly if detonation-driven combustion can be realized in supersonic combustible mixtures of scramjet combustors, because of the inherent theoretical advantage of detonation over deflagrative combustion [1-2].

On the basis of the detonation-driven scramjet (DDS) [3], a series of investigations [4-6] have been carried out on detonation initiation and propagation in supersonic channels using a hot jet initiation. It is globally found that to maintain dynamic stabilization of detonation in supersonic combustors is a great challenge. Lu and Braun [7] have reported that for practical detonation-driven engines it is a key issue to be able to sustain a detonation wave in the combustor for a long duration when bringing the concept to reality. In order to realize the DDS, quasi-steady propagation of

detonation in supersonic flows is one of the most important problems that need to be addressed.

Detonation is a supersonic wave coupled with reaction zone that propagates normally at an average CJ velocity. Therefore, it is very critical to dynamically stabilize the detonation in supersonic combustors with limited length when it propagates at the CJ state. Based on the idea of detonation stabilization in supersonic flows, several investigations have been carried out. First, enlightened by the outstanding performance to stabilize combustion of cavities normally used as flameholders in supersonic combustors [8-10], the cavity has been adopted for dynamical detonation stabilization in supersonic channels [11-12]. It is reported that the cavity can accelerate detonation propagation in supersonic channels, thus finally resulting in overdriven detonation due to the enhancement of pressure oscillations resulting from subsonic combustion in the cavity [11]. Especially owing to the detonation wave interaction with cavity a periodical process which consists of forward propagation, detonation attenuation and detonation self-sustainment, is generated to avoid detonation failure [12]. Second, considering that the actual combustors are usually expanding for thrust propulsion, recently two-dimensional detonation simulations have been conducted in supersonic expanding channels [5]. It is found that detonation sustainment can be maintained almost in the same position in the supersonic expanding channel after the shutdown of the hot jet. It is suggested that quasi-steady propagation of detonation can be achieved in the supersonic expanding channel for the given expansion angle. However, normally the dynamically steady state of detonation can only be maintained for a limited time, after which the detonation may gradually attenuate and finally fail because of the Prandtl-Meyer expansion fan resulting from the expanding wall.

Therefore, extra applicable approaches are very necessary to be cooperated together to effectively address the detonation stabilization problem in supersonic channels. In order to effectively realize the continuous quasi-steady mode of detonation propagation, in the present work detonation simulations are conducted in the supersonic expanding channels with a cavity embedded, where the combined effects of the expanding wall and cavity will both be explored on the dynamical stabilization of detonation.

It should be noted that both the cavity and expanding wall configurations can result in the generation of unburned jets, the consumption and subsequent heat release of which are subjected to rapid turbulent mixing and diffusion [6]. Radulescu et al. [13] has reported that the absence of small-scale turbulent interactions, normally not properly accounted for in detonation simulations, leads to significantly lower burning rates than observed experimentally and does not permit detonation self-sustainment. In the present work, the reactive Navier-Stokes (NS) equations with a simple reaction model [14] are solved using a high-order hybrid WENO-CD (Weighted Essentially Non-Oscillatory-Centered Difference) scheme [15-16] utilizing the open-source program AMROC [17-19] (Adaptive Mesh Refinement Object-oriented C++) based on an SAMR (Structured Adaptive Mesh Refinement) framework. The overall approach combines the robustness of WENO for discontinuity capturing with the benefit of a centered scheme with low numerical dissipation in smooth solution regions and the efficiency of SAMR. Therefore, the utilization of the NS equations and the low-dissipation hybrid high-order scheme associated with the SAMR is able to ensure the proper resolution of these small-scale turbulent interactions for more accurate physical descriptions when unburned jets are generated in supersonic flows. This work is part of an ongoing research program, aiming at providing information to help improve the overall understanding of dynamical stabilization of detonation in supersonic flows.

The remainder of this paper is organized as follows: Section 2 introduces the computational model, including governing equations, numerical methods and computational setup. Results and analysis are presented in Section 3, where quasi-steady propagation of detonation in supersonic expanding channels with a cavity, the subsequent stabilization mechanism and the influence of incoming velocities on quasi-steady propagation are further investigated. Finally, Section 4 concludes the paper.

2. Computational model

2.1. Governing equations

The present work utilizes the two-dimensional NS equations with a one-step two-species chemistry model as governing equations [6]. The simplified chemistry model [19] is selected and fitted to physical parameters of a H_2/O_2 detonation at $T = 300$ K and $P = 6670$ Pa with the corresponding CJ velocity of $V_{CJ} = 1587.84$ m/s, which are shown in Table 1.

Table 1 Thermodynamic parameters of the mixture.

Parameters	Values	Unit
T_∞	300	K
p_∞	6.67	kPa
ρ_∞	0.077552	kg/m ³
γ	1.29499	
W	0.029	kg/mol
q	54000	J/mol
E_a	30000	J/mol
A	6×10^5	s ⁻¹

The temperature and pressure at the end of the ZND reaction zone are approximately 2500 K and 1.01325×10^5 Pa respectively, which gives the following transport parameters for the reaction model: $T_{ref} = 2500$ K, $\mu_{ref} = 1.07 \times 10^{-4}$ Pa·s, $k_{ref} = 0.148$ W/(m·K), $D_{1ref} = 5.5 \times 10^{-4}$ m²/s, $D_{2ref} = 6.4 \times 10^{-4}$ m²/s. The viscosity, conductivity and mass diffusivity are selected by matching the general trends and values at the end of the ZND reaction zone between the simplified and detailed reaction model. The Sutherland model is utilized for the viscosity and conductivity while the mass diffusion values are derived from a simple expression which includes the inverse dependence on pressure.

2.2. Numerical methods

In the present work, the adopted hybrid WENO-CD scheme consists of two components: a finite-difference sixth-order WENO scheme to be used at discontinuities and a conservative sixth-order CD scheme for smooth-solution regions. Typically shock-capturing methods introduce excessive numerical dissipation, which pollutes the diffusive part of the NS equations; however, the methods which can discretize the diffusive terms without numerical dissipation usually lack robustness and stability at discontinuities. WENO schemes perform well for first-order hyperbolic problems, but introduce plenty of numerical dissipation for second-order mixed equations with physical diffusion. Meanwhile, no numerical viscosity is introduced for schemes developed with centered stencils, but generally numerical instabilities are produced at discontinuities. Therefore, through a switch based on a shock-based detection technique [20], the hybrid WENO-CD scheme can combine both the advantages of WENO and CD schemes: regions of strong discontinuities are approximated by the WENO scheme, while the CD scheme is used within regions of smooth flow, thus minimizing numerical dissipation to the extent possible, which has been demonstrated in the previous works [5][16].

Because of the stability properties of explicit integration schemes, the preferred practical methods with the ability of inexpensive time adaptation in SAMR are Runge-Kutta methods of third or higher order. In the present work, the optimal third-order strong stability preserving (SSP) Runge-Kutta scheme is used in combination with time-splitting and the fourth-order accurate semi-implicit GRK4A (A-stable generalized Runge-Kutta method of fourth order) method [19] for source term integration.

2.3. Computational setup

As depicted in Fig.1, the length and height of the channel are $X1 = 75$ mm and $Y1 = 25$ mm, respectively. The width of the hot jet is $X2 = 4$ mm, the distance from the hot jet to the front edge of the cavity is $X3 = 5$ mm, and the distance from the rear edge of the cavity to the outflow boundary is

$X_4 = 15 \text{ mm}$.

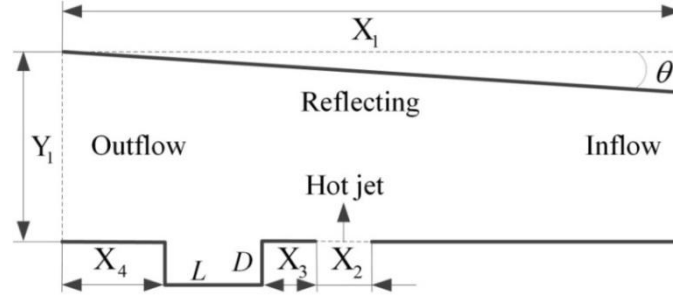


Fig.1 Schematic sketch of the calculation model.

The level-set technique for chemically reactive flows [17] is employed for the upper expanding channel section. Reflecting boundaries with slip-wall conditions are used on the upper and lower walls. At the lower wall boundary, a small inflow condition is set up to model a hot jet. Downstream in the hot jet is a cavity with the corresponding width and depth of $L=20 \text{ mm}$ and $D=10 \text{ mm}$ respectively. It is reported that a division between shadow and deep cavities is $L/D \cong 1$ [21]. When $L/D > 1$, the cavities may be considered shallow while when $L/D < 1$, the cavities may be considered deep. Therefore, the cavity is considered as a shadow one. Throughout the channel the supersonic reactive flow propagates from right to left at the corresponding CJ velocity. The right boundary adopts the inflow condition and an ideal outflow condition is imposed on the left boundary.

The inflow parameters of the hot jet are set to the values of the CJ state of a H_2/O_2 detonation under the condition of pressure 6.67 kPa and temperature 300 K . The injection velocity is given as the sonic speed to make it a choked one. The detailed information of the hot jet is shown in Table 2. In order to control the injection duration of the hot jet, the parameter "time" is also considered when dealing with the boundary condition. After detonation initiation is realized successfully, the hot jet is switched off and the inflow condition is immediately changed to the reflecting condition.

Table 2 The equilibrium CJ state of the hot jet. Note that the parameters for the species are given the mass fractions.

Parameters	Values	Unit
Pressure	86376	Pa
Temperature	1943.8	K
Density	0.155	kg/m^3
Velocity	850	m/s
Energy	349280	J/mol
Y_1	0.0088	
Y_2	0.9912	

2.4 Grid resolution

For the SAMR implementation, a five-level refinement strategy is utilized with refinement factors 2, 2, 2, 2 on the base mesh of 600×200 cells. As a result, the highest grid resolution of $\Delta_{\min} = 7.8 \times 10^{-6} \text{ m}$ can be obtained, which is the same with that utilized in the recent work [5]. In order to properly resolve the diffusion effect for unburned jets in the present work, the diffusion scales are considered. Among the three diffusive scales (viscous shear layer, thermal heat conduction layer and

mass diffusion layer), the viscous scale is the smallest, suggesting that a fully resolved simulation should be only limited by the viscous scale. Using the highest grid resolution, it is evaluated that at least about 10 cells can be placed within the viscous scale, hence indicating that these diffusive scales can be effectively resolved in the present simulations. It should be noted that, two-dimensional high-resolution computations would represent turbulent structures not necessarily correctly as vortex stretching is omitted in two dimensions, thus pseudo-DNS being performed.

3. Dynamic detonation stabilization

3.1 Detonation initiation

The initial expansion angle of $\theta = 4^\circ$ is employed for the expanding wall. In order to have a quick understanding of detonation initiation in the supersonic expanding channel with the cavity, a brief introduction is provided here in Fig.2.

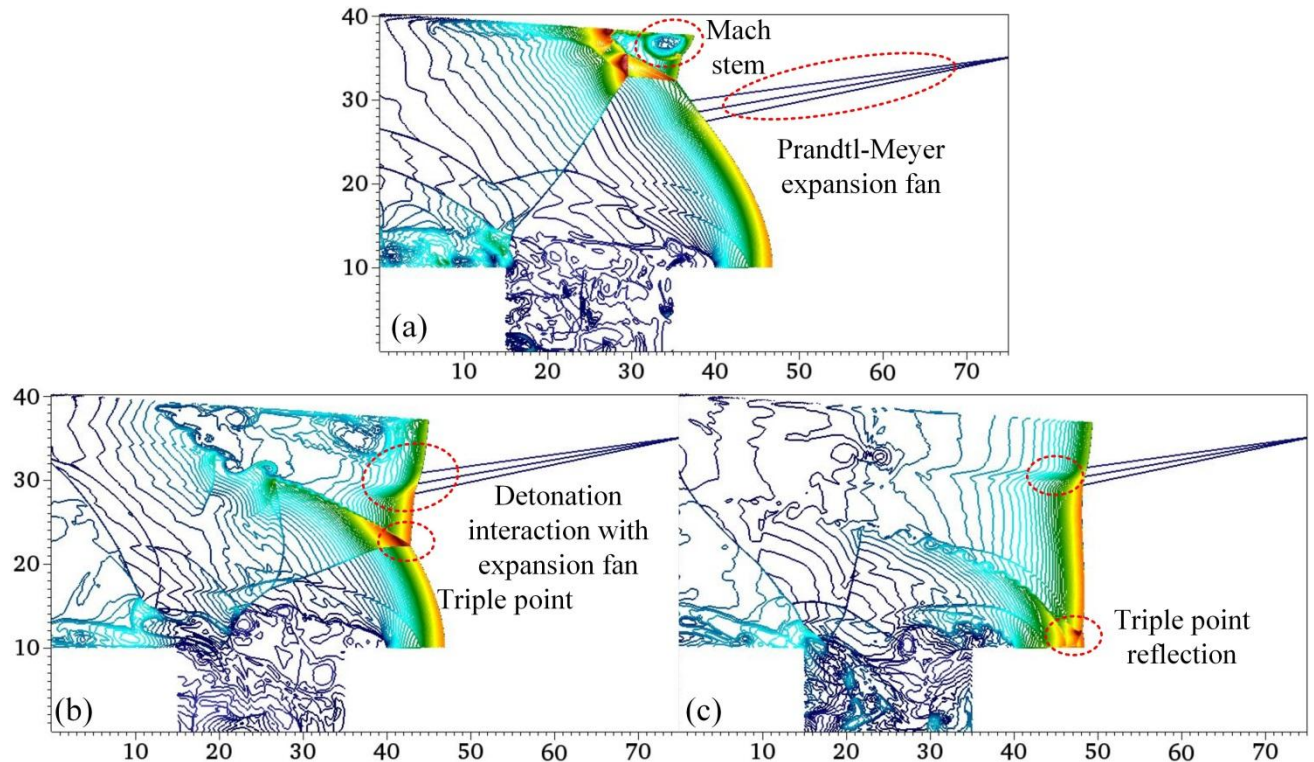


Fig.2 Density isolines showing the initiation process in the supersonic expanding channel with the cavity, (a) $t = 240 \mu\text{s}$; (b) $t = 270 \mu\text{s}$; (c) $t = 300 \mu\text{s}$

The time interval of the three successive frames is the same, denoted as $\Delta t = 30 \mu\text{s}$. After the injection of the hot jet into the channel, a bow shock is induced and subsequently reflects on the upper expanding wall. As shown in Fig.2(a), with the gradual strength increase of the bow shock, a Mach stem is generated, which has been demonstrated to be a local Mach detonation (Mach stem induced detonation) [22]. Due to the baroclinic vorticity production mechanism [13], the flow behind the Mach stem undergoes the RM (Richtmyer-Meshkov) instability, thus resulting in the formation of a Mach detonation bifurcation. This Mach detonation propagates toward the supersonic incoming flow with a velocity of V_{CJ} , suggesting that it is actually an overdriven detonation. With further forward propagation, the Mach detonation interacts with the Prandtl-Meyer expansion fan, as shown in Fig.2(b). Together with the forward propagation of the Mach detonation, the triple point propagates downward along the bow shock. As shown in Fig.2(c), the triple point has reflected on the lower wall and turns to propagate upward again, thus beginning a new period in the channel. The triple point reflection, which can immediately produce substantive heat release, contributes significantly to detonation self-sustainment in the supersonic flow.

3.2 Steady propagation of detonation

It is reported that overdriven detonation can be generated in supersonic channels due to the contractive passway mechanism resulting from the continuous hot jet injection [23]. Therefore, in order to investigate dynamically quasi-steady propagation of detonation in the supersonic expanding channel with a cavity, the hot jet is shut down at $t=130 \mu\text{s}$ after the initiation is fully realized in the supersonic flow to avoid the formation of contractive passway mechanism.

Fig.3 shows detonation propagation in the supersonic expanding channel with the cavity. It is observed that a small unburned jet is generated behind the detonation front due to the interaction of the Mach detonation with the Prandtl-Meyer expansion fan, as shown in Fig.3(a). A detached shear layer is generated near the unburned jet owing to the triple point collision on the expanding wall. At this moment, only one triple point is observed on the detonation front. Although the hot jet is shut down, the detonation still continues its forward propagation for a while until it eventually reaches the farthest position approximately at $Y=58.6 \text{ mm}$, where the hot jet effect can be considered as fully dissipated, as shown in Fig.3(b). During this period, the detonation wave begins to attenuate gradually, thus leading to the weaker detonation which results in the generation of multiple secondary triple points. Different from Fig.3(a), at least three secondary triple points are observed on the detonation front. Maxwell et al. [24] has reported that the triple point is not only a source of high temperature and pressure due to shock compression from multiple waves, but also a source of enhanced turbulent mixing. These triple points can give rise to slip lines further developed into shear layers that are susceptible to the KH instability [25-26], which thus act to enhance turbulent mixing between unburned pockets and burned gases [27-28]. It is found that near the expanding wall numerous large-scale vortices are produced due to the interaction between the unburned jet and highly unstable shear layers emitting from secondary triple points. Note that, some partly unburned pockets are even observed away from the detonation front after the separation from the main unburned jet. These large-scale vortices can enhance the turbulent mixing between the unburned pockets and burned product, thus facilitating the consumption of the unburned pockets.

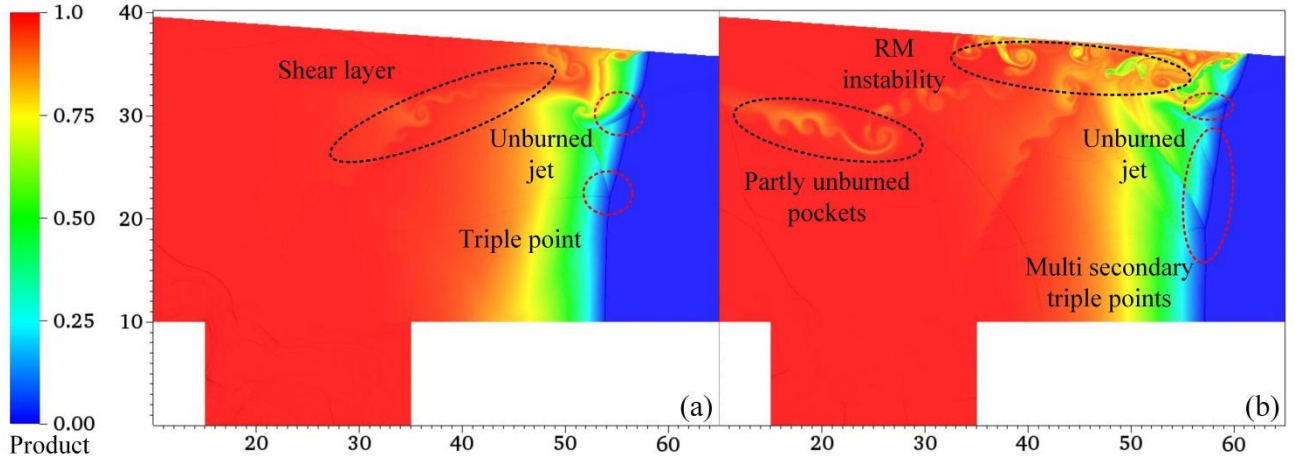


Fig.3 Detonation evolution after the shutdown of the hot jet, (a) $t = 345 \mu\text{s}$; (b) $t = 405 \mu\text{s}$

Globally, the Reynolds number ($\text{Re} = \frac{\rho avt}{\mu}$) is estimated using the average density, pressure

and temperature at the top and bottom of the shear layer behind the triple point while the time when the shear layer begins to become unstable is used. Here, the Reynolds numbers in Fig.3(a) and (b) are approximated as 5×10^4 and 1×10^5 , respectively. Dimotakis [29] has reported that 105 is an order of magnitude larger than the typical value for the onset of turbulence in mixing layers. Therefore, it is believed that after the shutdown of the hot jet the flow field around the unburned jet associated with the highly unstable shear layers behind the detonation front is in the turbulent regime after the detonation wave reaches the farthest position, which is beneficial for the turbulent mixing in the consumption of the unburned jet compared with the laminar mixing.

Fig.4 illustrates the trajectory of the detonation front, where the slope of the trajectory curve after the shutdown of the hot jet can represent the relative propagation velocity. Although the

injection of the hot jet ceases at $t = 310 \mu\text{s}$, it is found that the detonation continues the forward propagation until the farthest position is reached at about $t = 400 \mu\text{s}$. Subsequently, the detonation undergoes a slight backward propagation together with limited attenuation. Then, at $t = 600 \mu\text{s}$ the trajectory curve globally begins to exhibit a straightforward trend of horizontal line associated with periodical oscillations of an approximate period $\Delta T = 30 \mu\text{s}$, indicating that dynamical quasi-steady propagation of detonation is eventually realized in the supersonic expanding channel with the cavity. It should be noted that, for the given configuration in the present work, the detonation wave is dynamically stabilized at approximately $X=57 \text{ mm}$. It has been reported that in expanding channels variations of the expansion angle can change the corresponding expansion ratio which has influence on the characteristics of the expansion fan, hence leading to different nonuniform distributions of unreacted mixtures [5], while in channels with cavity embedded the cavity size can play a significant role in detonation propagation in supersonic combustible mixtures [12]. Therefore, it is suggested that the specified stabilization location is supposed to be dependent on the expansion angle, the cavity size, et al.

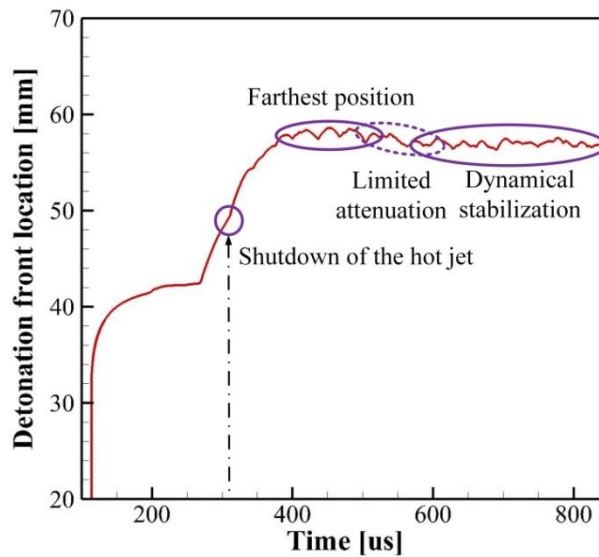


Fig.4 The trajectory of the detonation front in the expanding channel with the cavity

As shown in Fig.5, the successive four frames with the same time interval of $\Delta t = 10 \mu\text{s}$ properly illustrate the dynamical quasi-steady detonation propagation within one period. During the dynamic stabilization, near the expanding wall the structure of shock-induced combustion is generated for the four frames, as shown in Fig.5(a). Behind the shock-induced combustion are a series of large-scale vortices which are actually partly unburned pockets separated from the unburned jet. Besides, two main triple points can be observed in the detonation front, which propagate downward the lower wall. Therefore, the overall stabilization configure is a combination of the detonation wave in the lower part and shock-induced combustion in the upper part. After further propagation, the triple points begin to propagate upward after the collision on the lower wall and a small unburned jet is clearly observed at this moment as shown in Fig.5(b), which is larger than that in Fig.5(a). The large-scale vortices near the expanding wall is further dissipated due to the diffusion and mixing effects compared with that in Fig.5(a), and becomes nearly fully disappeared in Fig.5(c). Owing to the triple point collisions detached shear layers are generated and subsequently interact with the large-scale vortices. With its extension of the newly generated unburned jet, numerous vortices are produced along the unburned jet due to the KH instability as shown in Fig.5(d). These vortices will gradually become large-scale after the interaction with the highly unstable shear layers emitting from secondary triple points and can effectively separate the unburned jet into partly unburned pockets, which is similar with that in Fig.5(a). This can facilitate the consumption and further heat release of the unburned jet through the diffusion and mixing effects enhanced by the large-scale vortices. Results given in Fig.5 actually illustrate a fully periodic process of dynamically quasi-steady propagation of detonation in the supersonic expanding channel with the cavity.

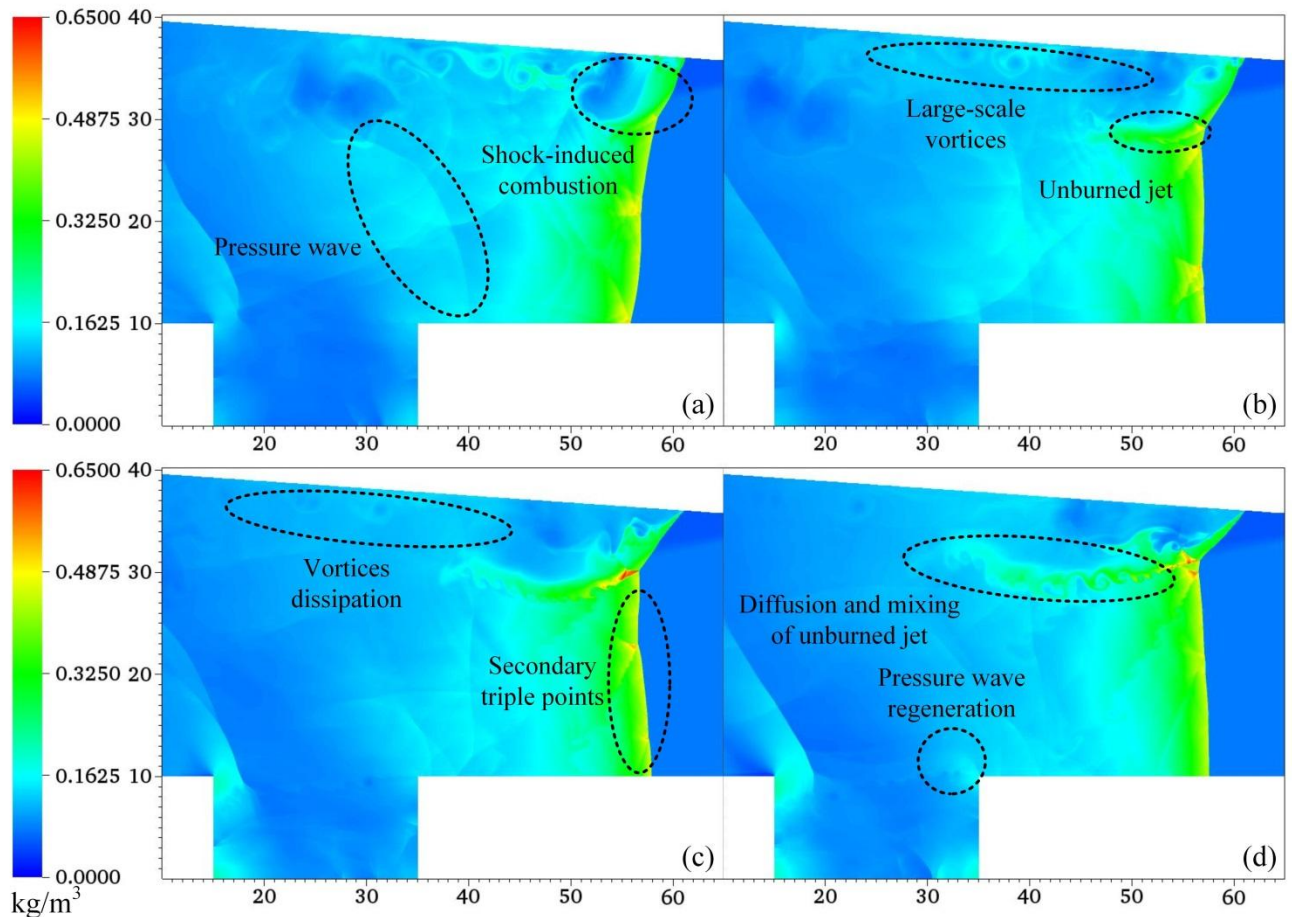


Fig.5 Dynamical quasi-steady detonation within one period, (a) $t = 730 \mu\text{s}$; (b) $t = 740 \mu\text{s}$; (c) $t = 750 \mu\text{s}$; (d) $t = 760 \mu\text{s}$

3.3 Stabilization mechanism

Usually, in supersonic straight channels, the detonation wave begins its gradual attenuation process associated with continuous backward propagation when the influence of the hot jet is totally dissipated [23]. However, as illustrated above in this supersonic expanding channel with the cavity embedded, the detonation wave quickly realizes dynamical stabilization when it arrives at the farthest position. Therefore, it is speculated that the expanding wall and cavity can both contribute to the realization of dynamical detonation stabilization.

However, simply through the dynamically quasi-steady propagation of detonation presented in Fig.5, it is difficult to figure out what roles the expanding wall and cavity can play in detonation stabilization in supersonic flows. Therefore, in order to ensure the actual combined effect resulting from the expanding wall and cavity on the dynamically quasi-steady propagation of detonation, two comparison cases are carried out. Both the two cases utilize the same condition, except for the difference that Case 1 uses a straight channel only with a cavity embedded while Case 2 employs a pure expanding channel without the cavity.

Fig.6 shows the trajectories of the detonation front for the two cases. For Case 1, after the shutdown of the hot jet, the slope of the trajectory curve first undergoes a very slight decrease due to the gradual dissipation of the hot jet effect, indicating the continuous forward propagation of detonation with a slight velocity decrease. When the hot jet effect is totally vanished, the trajectory exhibits periodical oscillations, but presents an overall constant slope as a whole, suggesting the eventual overdriven state of detonation. The relative velocity of forward propagation represented by

the constant slope, is calculated as $\Delta v = 161.7 \text{ m/s}$ with the corresponding overdrive degree of $f = 1.21$ ($f = (\frac{V_{CJ} + \Delta v}{V_{CJ}})^2$). The oscillation period is evaluated as $\Delta T_{Case 1} = 30.4 \mu\text{s}$ which is nearly the same with that in the expanding channel embedded with the cavity, indicating that the expanding wall does not have significant influence on detonation oscillations. Different from Case 1, the trajectory in Case 2 illustrates an overall different trend. After the shutdown of the hot jet, although the slope of the trajectory curve initially maintains a positive value, it turns to negative at $t = 340 \mu\text{s}$ after going through a short period of attenuation implying that the forward propagation of detonation changes to backward propagation quickly under this condition.

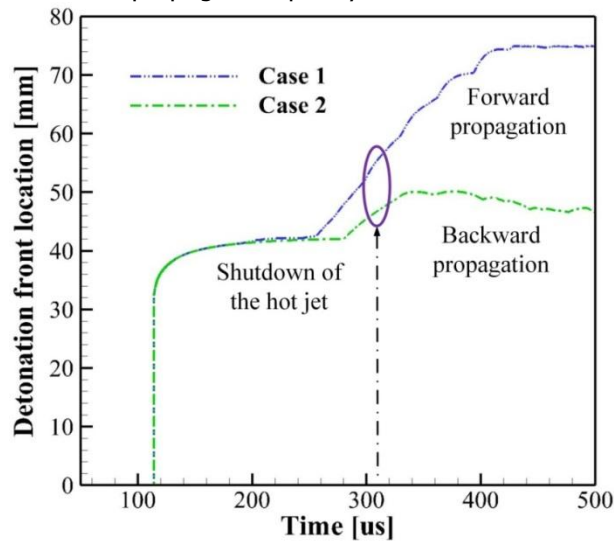


Fig.6 The trajectories of the detonation front for the two comparison cases

It has been demonstrated [12] that in supersonic combustible mixtures the acoustic wave produced by the subsonic combustion in the cavity can accelerate detonation propagation after crossing through the subsonic channel in the vicinity of the cavity edge, which can result in an overdriven detonation. This is also true in the supersonic expanding channel with the cavity, as demonstrated in Case 1. In the supersonic expanding channel, through the periodical formation and rapid consumption of the unburned jet resulting from the Prandtl-Meyer expansion fan, the detonation wave can be maintained almost in the same position [5]. However, with the increase of the expansion angle (e.g., the initial expansion degree of 40°), the unburned jet becomes enlarged so that much time is required for the jet consumption and the subsequent heat release. When the unburned jet is even extended out of the sonic line, the deficit of heat release cannot contribute to the quasi-steady propagation of detonation [30], thus eventually leading to detonation attenuation and even failure.

4 Conclusions

In the present work, dynamical detonation stabilization of supersonic combustible mixtures in expanding channels with a cavity embedded, is investigated solving the reactive NS equations and a one-step two-species reaction model using the hybrid sixth-order WENO-CD scheme based on the SAMR framework. The main results show that dynamically quasi-steady propagation of detonation can be realized in the supersonic expanding channel with the cavity during the backward propagation after the shutdown of the hot jet. The overall configuration of the dynamically stationary detonation is actually a detonation bifurcation consisting of the detonation wave and shock-induced combustion. In the supersonic expanding channel with a cavity, the quasi-steady propagation of detonation can be properly realized due to the two different effects: the one that can facilitate detonation propagation due to pressure oscillations resulting from the cavity and the other that can lead to detonation attenuation due to the Prandtl-Meyer expansion fan in the supersonic expanding wall, respectively.

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