Mechanism for Dynamical Stabilization of Detonation in Expanding Channels

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1 Introduction

Scramjets have become one of the first choices for hypersonic air-breathing propulsion systems thanks to the superior performance at high Mach numbers (Ma \geq 5.0) [1]. Scramjet combustors adopt the Brayton cycle, whose thermodynamic efficiency is much lower than that of detonation combustion [2]. It is expected that the performance of scramjets might be improved significantly if detonation combustion can be fully or even partially realized inside the scramjet combustor.

Based on the idea of detonation-driven scramjet, we have conducted a series of numerical investigations [3-7] on detonation initiation and propagation using a hot jet in supersonic combustible mixtures, where the open-source program AMROC [8-11] on an SAMR framework [12] is utilized. These numerical simulations solve the inviscid reactive Euler equations and apply a classical second-order accurate MUSCL-TVD scheme. It should be noted that these simulations are all carried out in simplified straight channels. Considering that the actual scramjet combustors are usually expanding for thrust propulsion, understanding the behavior of detonation in expanding channels is important for detonation physics and practical applications.

Recently, we computed two-dimensional high-resolution detonation simulations in expanding channels [13] using the reactive Navier-Stokes (NS) equations with a robust high-order hybrid WENO-CD scheme together with the SAMR framework. Although it is speculated that the detonation front can be maintained almost in the same position in the expanding channel through the periodical formation and rapid consumption of the unburned jet, the intrinsic mechanism for stabilization of detonation in expanding channels is still not well understood. In addition, it is noted that if the expanding angle is large enough, the detonation speed may not increase monotonously, and even detonation initiation might not be realizable, anymore, which also needs further study.

Following the previous study [13], in the present work, we solve the reactive NS equations with a simple reaction model [11] for detonation simulations in expanding channels with supersonic combustible mixtures by utilizing the high-order hybrid WENO-CD scheme together with the SAMR framework. This work is part of an ongoing research program, aiming at providing information to improve the overall understanding of detonation combustion in supersonic combustible mixtures.

2 Computational model

2.1 Governing equations

The two-dimensional NS equations with the one-step two-species chemistry model are utilized as governing equations. The simplified chemistry model is selected and fitted to physical parameters of a H_2/O_2 detonation at T = 300 K and P = 6670 Pa. Matching the general trends and values at the end of the ZND reaction zone between the one-step and detailed reaction model, the viscosity and conductivity values are obtained from the Sutherland model, and the mass diffusion values are derived from a simple expression which includes the inverse dependence on pressure.

2.2 Numerical method

Originally developed for large eddy simulations (LES) of turbulence, the hybrid WENO-CD scheme utilized here combines the advantages of both WENO and CD schemes. It is made up 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. The optimal third-order strong stability preserving (SSP) Runge-Kutta (RK) scheme is used with a CFL parameter 0.99 in combination with the fourth-order accurate semi-implicit GRK4A method for source term integration. The second-order Strang splitting method is used together with the third-order SSPRK due to the large difference in time scales between fluid dynamics and reactive source term.

2.3 Computational setup

Detonation simulations are conducted in two-dimensional expanding channels, as depicted in detail in Fig.1.



Figure 1. Schematic of the calculation model

The level-set technique with ghost fluid approach [9] is employed for the expanding upper boundary. Reflecting boundary with slip wall conditions are used on the upper and lower walls, and the inflow of the hot jet is embedded within the lower domain boundary. Throughout the paper the supersonic flow of the reactive mixture is from right to left at V_{CJ} ($V_{CJ} = 1587.84$ m/s). The right boundary adopts the inflow condition and an ideal outflow condition is imposed on the left boundary. Table 1: The ZND state of the hot jet. Note that the parameters for the species are given the mass fractions.

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Parameters	Values	Unit
Pressure	86376	Ра
Temperature	1943.8	Κ
Density	0.155	kg/m ³
Velocity	850	m/s
Energy	349280	J/mol
\mathbf{Y}_1	0.0088	
\mathbf{Y}_2	0.9912	

The inflow parameters of the hot jet are set to the values of the ZND state of a detonation in H_2/O_2 under the condition of the inflow pressure 6670 Pa and the temperature 300 K, as shown in Table 1.

3 Results and analysis

As for the expanding channel, the expansion angle of $\theta = 3^{\circ}$ is initially considered here. After initiated in the expanding channel, overdriven detonation is generated due to contractive passway mechanism [6] induced by the hot jet. After the shutdown of the hot jet, it is reported that the detonation front can maintain its quasi-stable state even in the expanding channel [13]. In order to have a quick understanding of this issue, a very brief illustration is provided here.

3.1 Detonation stabilization

Fig.2 illustrates detonation propagation in the expanding channel after the shutdown of the hot jet at $t = 350 \,\mu\text{s}$.



Figure 2. Dynamically stable propagation of detonation, (a) $t = 595 \,\mu\text{s}$, (b) $t = 605 \,\mu\text{s}$, (c) $t = 615 \,\mu\text{s}$, (d) $t = 625 \,\mu\text{s}$, (e) $t = 635 \,\mu\text{s}$, (f) $t = 645 \,\mu\text{s}$

It is observed obviously that the instability undergoes an increase on the detonation front on the whole. Fig.2(a)-(c) describes the generation process of an unburned jet directly behind the expansion fan due to a Prandtl-Meyer expansion. Fig.2(d)-(f) depicts the generation of a new unburned jet, indicating the formation of a periodical detonation evolution in the expanding channel.

Fig.3 records the locations of the detonation fronts near the lower and upper walls. When the hot jet is shutdown at $t = 350 \,\mu\text{s}$ the detonation front is almost maintained at the same position, and periodical oscillation is basically realized at $t = 500 \,\mu\text{s}$, indicating the formation of dynamically stable propagation of detonation.



Figure 3. Location records for the lower and upper detonation fronts, (a) with continuous hot jet injection (b) after hot jet shutdown

3.2 Stabilization mechanism

In expanding channels, the turbulent mixing between the unburned jet and highly unstable shear layers emitted from multi secondary triple points facilitates the consumption of the unburned jet. The accelerated periodical heat release through the rapid consumption of the unburned jet to some degree can compensate the additional attenuation effect resulting from the expansion wave in expanding channels.



Figure 4. Schematic sketch of hydrodynamic throat induced by the unburned jet

In addition, slip lines are generated due to the KH instability along the unburned jet, which are further developed to highly unstable shear layers associated with large-scale vortices. These slip lines can be considered as free boundaries, together making up of a hydrodynamic throat with the lower wall, as shown in Fig.4.

Therefore, the mechanism of stabilization of detonation in expanding channels can be concluded as follows. First, due to the turbulent mixing resulting from large-scale vortices along the unburned jet, generation and consumption of the unburned jet are enhanced for rapid periodical heat release, providing chemical energy for propagation maintenance. Second, due to the formation of hydrodynamic throat, further detonation attenuation is effectively suppressed.

4 Discussion

On the one hand, this can make the flow highly turbulent, thus facilitating the consumption of the unburned jet and the subsequent chemical heat release due to the enhanced turbulent mixing. However, on the other hand, the enlarged unburned jet needs to take more time for the full consumption. The existence of the enlarged unburned jet that get swept downstream can result in an increase in the

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effective length of the reaction zone of the detonation wave, and the delayed chemical heat release of the unburned jet cannot play any role in the detonation propagation if it is left behind the sonic plane.

Fig.5 shows typical flowfield structures for two expansion angles under the shutdown of the hot jet, in which the blue lines represent sonic boundaries. The majority of the unburned jet for the larger expansion angle cannot be combusted quickly, being left behind the sonic plane, although a stronger turbulent mixing effect is expected due to the generation of relatively larger vortices along the jet boundaries.



Figure 5. The flowfields for two different expansion angles under the shutdown of the hot jet, (a) expansion angle of 3° at $t = 665 \ \mu s$, (b) expansion angel of 8° at $t = 480 \ \mu s$

In addition, compared with Fig.5(a) and (b), it is indicated that due to the formation of the larger unburned jet, the shear layers along the jet become more highly unstable, thus resulting in more large-scale vortices. The intrinsic instabilities of these vortices increase the fluctuations of the shear layers considered as free boundaries, hence to some degree destroying the stable structure of the hydrodynamic throat which utilizes the shear layer as the top boundary. Nevertheless, the instabilities can enhance the consumption of the unburned jet due to the mixing effect resulting from large-scale vortices along the unburned jet, which can contribute to the detonation to be sustained when the chemical heat is released in front of the sonic location.



Figure 6. Detonation attenuation for the expansion angel of 8° under the shutdown of the hot jet, (a) $t = 560 \ \mu s$; (b) $t = 590 \ \mu s$

Fig.6 illustrates the latter period of detonation attenuation for the expansion angle of 8° after the hot jet shutdown. Near the upper expanding wall is the oblique shock-induced combustion with the

unburned jet generated underneath. Underneath the shock-induced combustion are the unburned jet and the Mach stem. Compared with Fig.6(a) and (b), it is observed that the reaction front is gradually separated from the Mach stem, indicating that the attenuation will eventually lead to detonation failure.

5 Conclusions

The mechanism of stabilization of detonation in expanding channels is investigated solving the reactive NS equations and one-step two-species reaction model using the hybrid high-order WENO-CD scheme based on the SAMR framework. The results show that generation and consumption of the unburned jet are enhanced for rapid periodical heat release due to the turbulent mixing resulting from large-scale vortices along the unburned jet, which can contribute significantly to propagation maintenance through chemical energy provision. In addition, further detonation attenuation is suppressed due to the formation of the hydrodynamic throat. These two effects combined together can lead to dynamical stabilization of detonation in expanding channels after the shutdown of the hot jet.

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