Numerical Investigation of H_2–O_2 Layered Detonation in Narrow Channel

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1 Introduction

The previous experiments[1] of scramjet engine with a hypermixer (HM) injector, which generates streamwise vortices for enhancing supersonic mixing and combustion, was examined in a Mach 8 simulated flight condition at High Enthalpy Shock Tunnel(HIEST) of JAXA, Japan. In equivalence ratio Φ = 1.0, 1.5, transient combustion wave, which propagates opposite direction to the main flow, were observed. The properties of pressure were well agreed with those of Chapman-Jouguet detonation wave, and indicate that this combustion wave was a kind of detonation wave. The mixing condition in the combustor was numerically investigated by Kodera *et al*[2]. The mixture has a gradient of fuel density in the cross-section in the combustor, where H_2 mole fraction was higher at the center and lower near the wall.

Detonation is a supersonic combustion wave propagating in a premixed gas. Its structure is composed by incident shock wave, Mach stem, transverse wave, and triple points. Layered detonation is a detonation, which propagates in layered premixed gas, and has been investigated by many researchers. The detonation wave that was observed in the experiments of HM injector seems a kind of layered detonation. Liu *et al*.[3] developed a special double-layer shock-tube to observe the complex interactions of a layered detonation experimentally. They performed a series of experiments using various gaseous combinations. Liu *et al.*[4], Liou *et al*.[5], and Fan *et al*.[6] analyzed these experiments and described several possible steady state by the theory of oblique shock and detonation polars. As for numerical simulations, Oran *et al*.[7] calculated a layered detonation in a large channel where cell structure does not effect to the dynamics of the flow field. They also showed a good agreement with experimental results, and described the dynamics of decay and reigniting process in detail.

The aim of this work is to numerically examine the characteristics of detonation and the effect of parameters in the layered mixture. The mixture consists of stoichiometric layer and non-detonable concentration layer. In the experiment of HM injector, the height of combustor was 12mm, and it is similar to the cell width. Therefore, this work is conducted in the narrow channel where the one cell appears to investigate the structures in the layered gases.

2 Numerical setup

The schematic of the computational domain in this work is shown in Fig. 1. Detonation is firstly developed in the uniform mixture, and then detonation propagates into the non-uniform mixture. At the non-uniform mixture, the gas has double layer in vertical direction. Equivalence ratio of upper

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layer is out of detonable concentration (lower than the detonation limit). The initial pressure P_0=1atm and temperature T_0=298K are used in both layers. The channel width W is 11$L_{1/2}$ in all cases. Important parameters in this work are non-detonable layer equivalence ratio ϕ' in upper layer and its width δ to examine the characteristics of the layered detonation. These values used in this work are listed in Table 1.

The governing equations are the compressible and reactive two-dimensional Euler equations for the calculations of the layered detonation. The fluid is a perfect gas, and all diffusions are neglected. In the current study, a 9-species, 19-reaction mechanism for hydrogen-air combustion[8] is used, and nitrogen molecule is included as an inert species. As discretization methods, Yee's Non-MUSCL Type 2nd-Order Upwind Scheme[9] is used for the spatial integration, and point-implicit method that treats only source term implicitly is used for the time integration.

The computational grid is an orthogonal system for two-dimensional calculations. In all calculations, at least 22 grid points in half reaction length $L_{1/2}$ are set in the vicinity of incident shock. The axial length in the computational grid is more than 100$L_{1/2}$ to avoid disturbance from the right boundary which is the non-reflected boundary proposed by Gamezo *et al*[10]. The left boundary is inflow condition, the upper is adiabatic slip wall, and lower is set mirror condition to imitate experimental condition.

3 Results

The propagation characteristic of the layered detonation on ϕ'-δ plane is shown in Fig. 2. The propagation limit of low-reactivity width δ increases monotonously as to the rise of ϕ'. Although all upper layer conditions are lower than the detonation limit, their reactivity in terms of the detonation propagation in the layered mixture highly depends on the concentration of non-detonable gas.

To clarify the mechanism of the wave propagation in the layered detonation, the time evolution of the flow fields of shock front in (a) uniform gas, (b) layered gas(maintain), and (c) layered gas(decay) are compared in Fig. 3. The shock front velocity and the maximum pressure at upper and lower boundaries are shown in Fig. 4. The time evolutions of transverse wave strength S are shown In Fig. 5. In Fig. 3(a) the transverse detonation(TD) strikes the upper and the lower boundaries alternately, and its strength is almost constant in Fig. 4(a). The propagation velocity has small variations during the propagation of transverse wave from upper to lower boundary. In Fig. 5(a), S increases monotonously when TD propagate upward and downward directions.

In Fig. 3(b), the transverse detonation fails after penetrating the upper low-reactive layer and becomes the transverse wave(TW). After coming back to the lower layer, the transverse wave is followed by the burnt area, and finally the transverse detonation is regenerated by the collision of the transverse waves at the lower boundary. In Fig. 5(b), S shows much particular mechanism. S decreased rapidly at t = 1.0 μs, when TD penetrate to upper layer. It indicates the transition from TD to TW. Afterwards, S decrease monotonously because of the separation of TW and reaction front, and increase discontinuously at t = 2.2 μs, when TW penetrate to the lower layer. It is because the rise of propagation speed of TW caused by the penetration of density discontinuous line(layered gas boundary). Thereafter, S decrease again even it is followed by the reaction front, and make drastic increase at t = 3.4 μs. It is caused by the regeneration of TD, and the maximum strength S = 4.2 is similar to the uniform gas condition. The periods of traveling time between the upper and lower boundaries in Fig. 4(b) says that the upward average velocity is much faster than the downward one. Furthermore, the history of the propagation velocity shows the detailed behavior during propagation. Comparing the velocity profile and the maximum pressure, the peak pressure at the lower boundary induces the rapid increase of the propagation velocity. Hence, the collision of the transverse waves at the lower boundary maintains the detonation propagation.

In Fig. 3(c), the transverse wave after traveling in the upper layer is not followed by the burnt area, and therefore the incident shock separates from the effect of the energy release and decays gradually. Fig. 4(c), the propagation velocity decreases monotonously and converges to about 1400m/s. In Fig.

5(c), S also decrease at t = 1.0 μs when TD penetrate to upper layer and increase at t = 2.4 μs when TW penetrate to the lower layer. At t = 4.0 μs when TW reflect to the lower boundary, S does not increase and then go down to zero. It indicates that any ignition was caused by the TW reflection. Hence, TW get weak as time goes by and detonation wave transit to plane wave.

Figure 6 is the histories of the propagation velocity of (a) ϕ' = 0.3, $\delta = 3L_{1/2}$, (b) ϕ' = 0.3, $\delta = 4L_{1/2}$, and (c) ϕ' = 0.3, $\delta = 5L_{1/2}$. The histories show the different behavior depending on δ, and therefore the average propagation velocity must be difference each other. Since the total heat release determines the detonation velocity, we calculated the average equivalence ratio ϕ_{av} for each condition. The average propagation velocity derived from the simulated result and the CJ velocities derived from the average equivalence ratio of the layered gas mixture are listed in Table 2. The average equivalence ratios are (a) ϕ_{av} = 0.775, (b) ϕ_{av} = 0.705, and (c) ϕ_{av} = 0.640.In conclusion, the propagation velocity in layered gas agrees well with the values estimated by average equivalence ratios for such a narrow channel layered detonation.

4 Conclusion

Detonation in the layered mixture, which consists of stoichiometric layer and non-detonable concentration layer in the narrow channel, was numerically investigated using two-dimensional Euler equations with H_2 - O_2 detailed reaction model. The reactivity of layered detonation had a strong relationship to the non-detonable layer concentration. When the layered detonation propagates, the transverse detonation became transverse wave in the non-detonable layer, and the collision of this transverse waves at the lower boundary maintained the propagation. Furthermore, The propagation velocity of layered detonation well agreed with the CJ velocity of the average equivalence ratio of layered mixture for a narrow channel.

Acknowledgement

This work was supported by Grant-in-Aid for Scientific Research(S) 21226020.

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Table 1. Using parameters

Parameters	value
Upper layer equivalence ratio ϕ'(mixture of H_2, O_2, N_2)	0.0 - 0.3
Width of upper layer δ	$1 - 11L_{1/2}$
Lower layer equivalence ratio ϕ (mixture of H_2, O_2, N_2)	1.0
Channel width W	$11L_{1/2}$

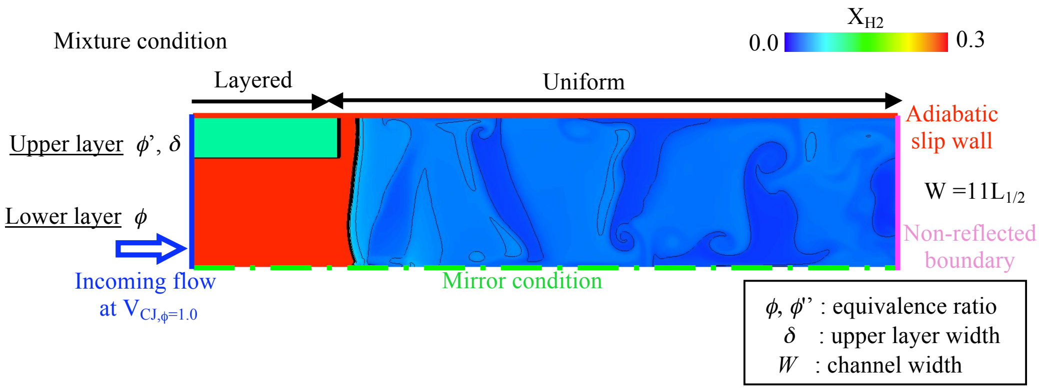


Fig. 1 schematic of the computational domain

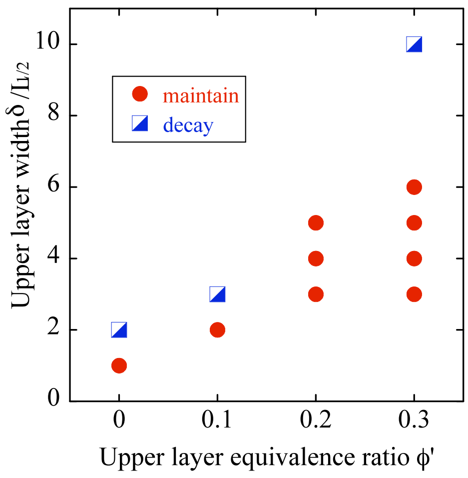


Fig. 2 The propagation characteristics of layered detonation as a function of low equivalence ratio ϕ' and its width δ.

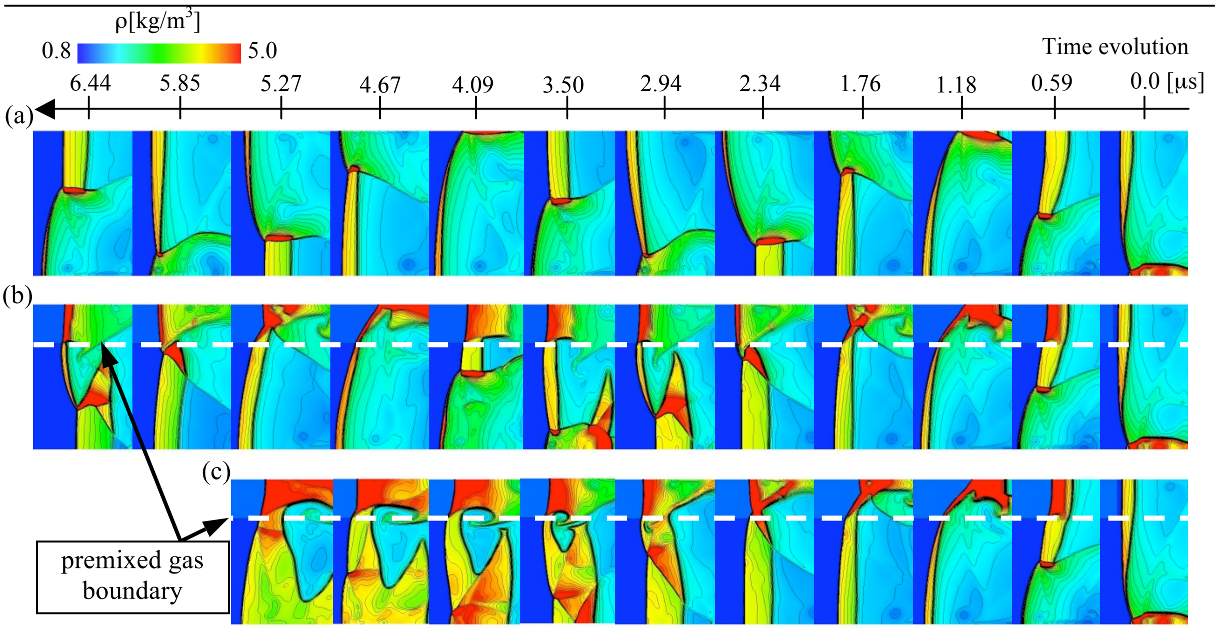


Fig. 3 The development of shock propagations (view is focused on the shock front)
(a) uniform (b) layered gas (maintain) ; ϕ'=0.3, δ=3$L_{1/2}$
(c) layered gas (decay) ; ϕ'=0.1, δ=3$L_{1/2}$

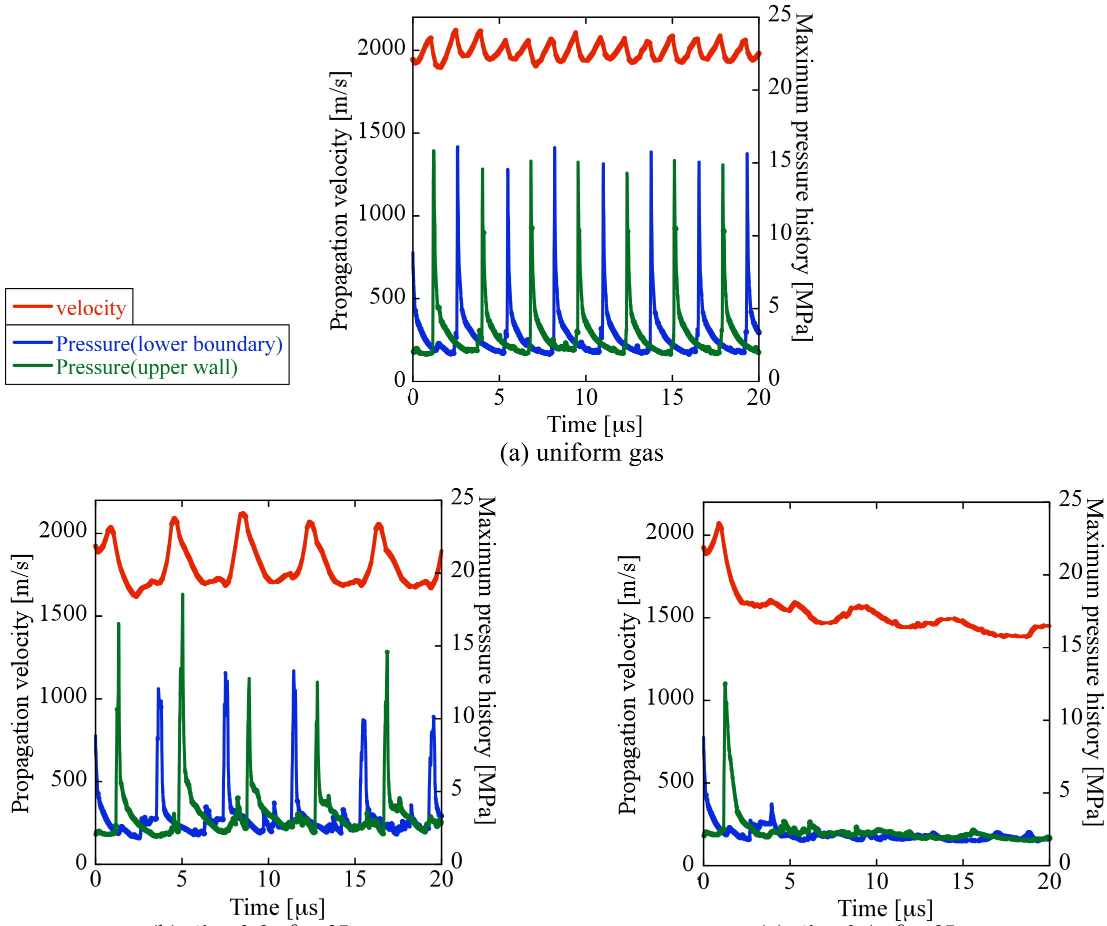
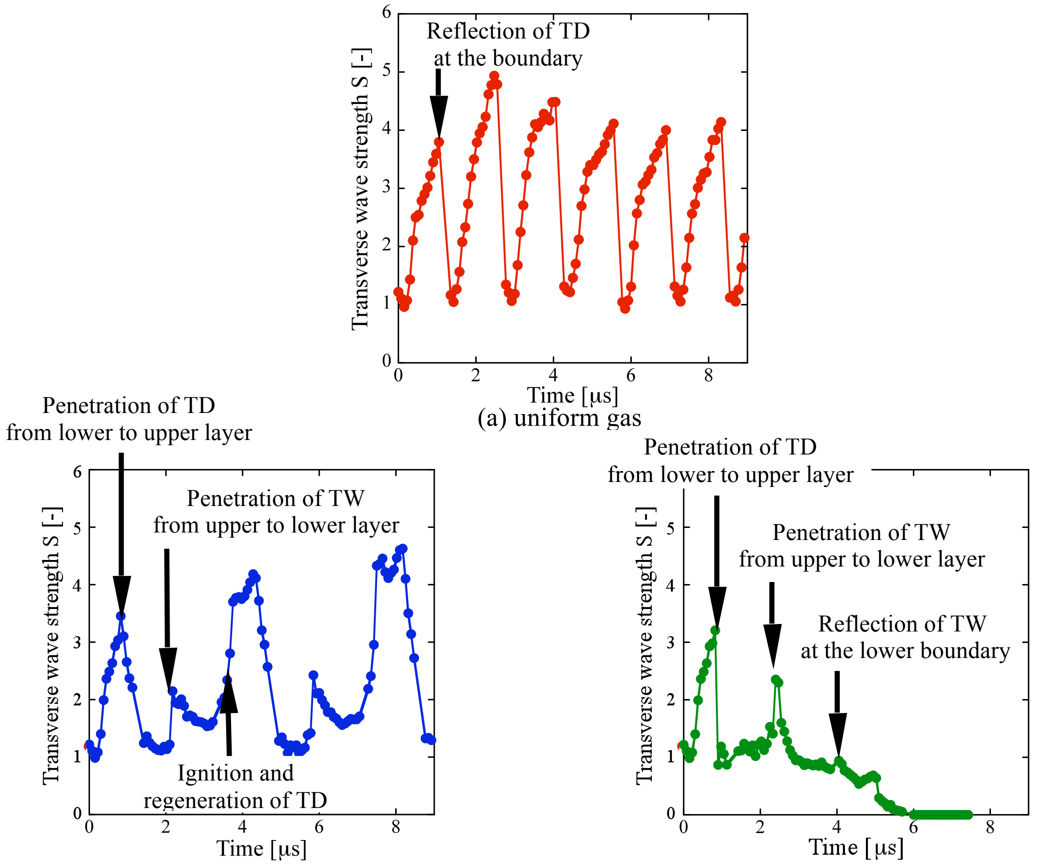


Fig. 4 The propagation velocity and maximum pressure history of upper and lower boundary
(a) uniform gas (b) layered gas (maintain) :ϕ' = 0.3 δ = 3$L_{1/2}$
(c) layered gas (decay) :ϕ' = 0.1 δ = 3$L_{1/2}$



(a) uniform gas

(b) ϕ' = 0.3, δ = $3L_{1/2}$ (c) ϕ' = 0.1, δ = $3L_{1/2}$

Fig. 5 The propagation velocity and maximum pressure history of upper and lower boundary
(a) uniform gas (b) layered gas (maintain) : ϕ' = 0.3 $\delta = 3L_{1/2}$
(c) layered gas (decay) : ϕ' = 0.1 $\delta = 3L_{1/2}$

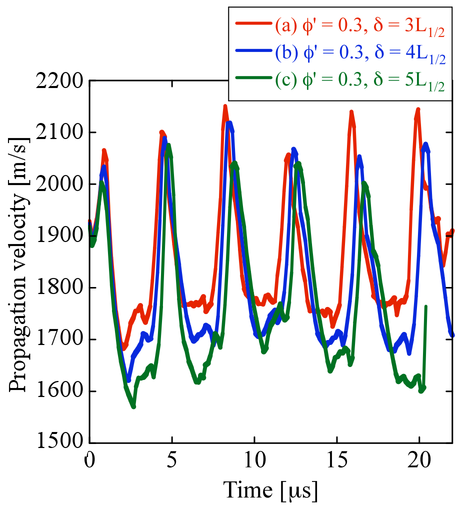


Fig. 6 The propagation velocity of layered detonation of ϕ' = 0.3 and (a) $\delta = 3L_{1/2}$, (b) $\delta = 4L_{1/2}$, (c) $\delta = 5L_{1/2}$

Table 2. Propagating velocity and predict value

	averaged propagation velocity D[m/s]	CJ velocity of average equivalence ratio $D_{\phi av}$[m/s]	average equivalence ratio ϕ_{av}
(a) δ = $3L_{1/2}$	1846	1848	0.775
(b) δ = $4L_{1/2}$	1807	1798	0.705
(c) δ = $5L_{1/2}$	1769	1745	0.640