Numerical Simulation on Two-Dimensional H_2 / Air Detonation Waves Propagating in a Converging-Diverging Nozzle

Hiroyuki Jotaki*, Nobuyuki Tsuboi, and A.Koichi Hayashi*****

*Dept. of Mech., Aoyama Gakuin Univ., 5-10-1 Fuchinobe, Sagamihara, Kanagawa 229-8558, Japan,

E-mail : jotaki@cow.me.aoyama.ac.jp

**Institute of Space and Astoronautical Science, Japan Aerospace Exploration Agency,

E-mail:tsuboi@flab.eng.isas.jaxa.jp

***Dept. of Mech. Eng., Aoyama Gakuin Univ., E-mail : hayashi@me.aoyama.ac.jp

1. Introduction

Detonation is the explosion phenomenon that chemical reactions are inducted by the preceding shock wave and propagates at a supersonic speed in a reactive gas mixture. Detonation generates much higher pressure than deflagration propagating at a slower speed than the sound speed. Detonation waves have been studied at a safety engineering point of view for over one–hundred twenty years and recently the application of detonation to the next generation propulsion devices is expected as Pulse Detonation Engine (PDE) [1] and Oblique Detonation Engine (ODE).

PDE generally consists of one closed end and another open end. Its exit opens to the atmosphere. At first, PDE tube is filled with fuel and oxidizer gas. Secondly, the mixture gas is ignited with a high energy ignition device near the closed end. Thirdly, the propagating deflagration overtakes the preceding shock wave and DDT occurs, and the detonation wave propagates towards the tube end, while high pressure is generated in the closed tube end. PDE is the propulsion system to produce thrust by the intermittent cycle. PDE combustion efficiency is higher than that of other chemical propulsion devices based on the constant-pressure cycle and PDE consists of a simpler structure, costs less, and is lighter than the traditional propulsion devices.

The tasks for developing applicable PDE are to be high cycle operation, efficient ignition device and fuel/oxygen injection method in order to reduce DDT length, increase high performance and high efficiency. These tasks are mainly conducted by experimental methods. Recent computational hardware remarkably develops and some of these tasks are studied by numerical methods. One of the efficient methods to increase PDE performance optimizes nozzle geometry; however, the past researches have been done in order to reveal detonation phenomena with a constant channel. Therefore, the detonation propagation in a nozzle for converging-diverging(C-D) type or other types has to be studied in detail [2], [3], [4]. Edwards [5] examined a diverging detonation wave generated by a two-dimensional nozzle filled with a detonable gas and obtained some information. However, the detailed mechanism of the detonation propagating through the nozzle is still unclear. Moreover, the detonation has many cells in its front and their effects are not estimated though the mechanism of quenching or re-initiation would be governed by the detonation cells.

This paper presents the fundamental study of detonation for PDE with a nozzle. In particular, we discuss the results of the numerical simulation with a detailed chemical reaction model for detonation waves propagating in the two-dimensional converging-diverging nozzle.

2. Numerical methods

The two-dimensional compressive Euler equations with a mass conservation law for each chemical species are integrated in this study. The second-order explicit Harten-Yee non-MUSCL modified-flux type TVD-upwind scheme is used for convective terms. A point implicit method is applied for production terms. Moreover, a second-order Strang-type fractional step method is used for a time integration. In this numerical condition the test gas is the stoichiometric gas mixture with hydrogen as a fuel and oxygen as an oxidizer and is diluted by argon gas or nitrogen gas. The former gas is $2H_2$+O_2+7Ar and the latter is $2H_2$+O_2+3.76N_2. The initial pressure is 101.3 kPa and its temperature is 298.15 K in both cases. The Chapman-Jouguet(C-J) detonation velocity in this condition is 1694 m/s in the gas diluted by Ar and 1971 m/s in the gas diluted by N_2.

In the present simulation the results of the two-dimensional C-J detonation are used as initial conditions for nozzle configurations. The two-dimensional detonation with a constant channel width is calculated in the first place. The number of grid points is about 660,000(3321x201). Figure 1 shows the computational grid system, where a grid point for every twenty points is plotted. There are 2521 points for the nozzle section among 3321 points at x-direction. In the case of the argon dilution the grid scale is dx=2.0 μm and dy= 2.0 μm in front of the nozzle section, at the nozzle entrance and at the nozzle exit. The grid scale at the throat is dx=0.2 μm and dy= 2.0xW_{throat}/W_{tube} μm. The computational domain is 3.2 mm in the propagating direction and 0.4 mm for the width of the tube. The length of the nozzle is 1.6 mm. In contrast, in the case of the nitrogen dilution, the grid scale is dx=5.0 μm and dy= 5.0 μm in front of the nozzle section, at the nozzle entrance and at the nozzle exit. The grid scale at the throat is dx=0.5 μm and dy= 5.0xW_{throat}/W_{tube} μm. The computational domain is 8.0 mm in the propagating direction and 1.0 mm for the width of the tube. The length of the nozzle is 4.0 mm. It is thought that a qualitative discussion about the propagating structure of detonation is possible though the calculation area is small due to maintaining the resolution. As for the chemical reaction model in this study, the detailed chemical reaction model developed by Petersen and Hanson [6] is used. This reaction model has 9 chemical species (H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, and N_2) and 18 elementary processes. The model features to include the pressure dependence in the tri-molecular collision reactions.

It is assumed in the boundary condition that the left closed end of the tube and the upper and lower walls are at adiabatic, non-catalytic, and slip, and the right boundary is open end. The exit pressure at the right boundary is 0.1 atm(external pressure) when the Mach number of the outflow at the exit is less than 1.0 and all are extrapolated when the Mach number of the outflow at the exit is larger than 1.0.

3. Results and Discussions

The present simulation estimates the phenomena of detonation waves propagating in hydrogen/oxygen (ϕ = 1.0) diluted by argon and nitrogen gas through converging-diverging nozzles with W_{throat}/W_{tube}=0.12, 0.50 and 1.00.

Figure2 shows the result of the maximum pressure history for the nozzle of W_{throat}/W_{tube}=0.12, 0.50 and 1.00, respectively. Figure 2-(a) is the case of the argon dilution and figure 2-(b) is that of the nitrogen dilution. These results present that in both Fig.2-(a) and Fig.2-(b), the trail of the triple point continues to the tube exit for the case of the nozzles with W_{throat}/W_{tube}=0.50 and 1.00, however it is confirmed that the trail disappears in the diverging section in the case of the nozzle with W_{throat}/W_{tube}=0.12. These results show that the detonation keeps its strength in the case of the nozzles with W_{throat}/W_{tube}=0.50 and 1.00, but that it becomes a deflagration in the case of the nozzle with W_{throat}/W_{tube}=0.12. The pressure near the triple point reflected on the wall becomes higher in the argon dilution than in the nitrogen dilution because the channel width in Fig.2-(a) is narrower in fig.2-(a) than that in Fig.2-(b) and the triple point is reflected on the wall with higher pressure. It is confirmed that there is a high pressure and temperature area near the nozzle throat in the converging section. This means the transverse wave strongly interacts with the wall. Moreover, the size of the high pressure and temperature area in Fig.2-(a) is wider than that in Fig.2-(b) due to chemical composition and thermodynamic property.

Figure 3 shows the results of the argon dilution and the nozzle with W_{throat}/W_{tube}=0.50. The instantaneous pressure contours are shown in Fig.3-(a) and the instantaneous temperature contours are shown in Fig.3-(b). In Fig.3-(a), the transverse wave reflects with the wall and it becomes parallel to the wall when the detonation front propagates in the converging section. In particular, this is clearly confirmed at t=0.66 μs in Fig.3-(a). After the detonation front propagates through the nozzle throat, the low pressure area appears near the upper and bottom wall in the diverging section near the throat due to the expansion at t=0.70 μs. As the detonation front propagates in the diverging section of the nozzle, this low pressure area expands. It is confirmed that the transverse wave is cut by this expansion wave as shown at t=0.78 μs in Fig.3-(a). At t=0.53 μs and t=0.62 μs in Fig.3-(b), the pressure between the transverse wave and the bottom wall is high. In contrast, after the triple point reflects on the upper wall, especially at t=0.78 μs in Fig.3-(b), the temperature between the transverse wave and the upper wall becomes high, but the temperature near the throat in the diverging section is not high. This agrees with the former description.

Figure 4 shows the results of the nozzle with W_{throat}/W_{tube}=0.12 and the argon dilution. The instantaneous pressure contours are shown in Fig.4-(a) and the instantaneous temperature contours are shown in Fig.4-(b). The phenomena shown in the detonation wave propagating in the nozzle with W_{throat}/W_{tube}=0.12 is basically similar to that occur in the detonation wave propagating in the nozzle with W_{throat}/W_{tube}=0.50. However, there are two differences between in the cases of the nozzle with W_{throat}/W_{tube}=0.12 and W_{throat}/W_{tube}=0.50. The first is that after the detonation front propagates through the nozzle throat, significant high pressure and temperature area appear near the throat. The flow behind the detonation front would stagnate or choke near the throat. The mass flow rate should be calculated to show the effects. The second is that when the detonation front propagates in the diverging section of the nozzle, at t=0.66 μs and t=0.76 μs in Fig.4-(a), (b), the triple point and transverse wave disappear near the wave front. This phenomenon is caused by the strong expansion near the throat and the strength W_{throat}/W_{tube}=0.12 is larger than that for W_{throat}/W_{tube}=0.50. In particular, at t=0.76 μs in Fig.4, low pressure and temperature areas expand at the right direction of the throat and the triple point is unclear near the wave front. The present results indicate that the detonation wave changes to deflagration through the throat.

Figure 5 shows the instantaneous detonation velocity histories along the nozzle center in the case of the argon dilution and figure 6 shows that in the case of the nitrogen dilution. These results are plotted in the nozzle section. The instantaneous rapid acceleration of the detonation velocity means that the triple point passes across the nozzle center. In the cases of both the argon and nitrogen dilution, the interval which the triple point passes across the center becomes short when the throat width becomes narrow. The averaged detonation velocity for W_{throat}/W_{tube}=1.00 is approximately C-J values, whereas that for the nozzle becomes an overdriven state in the converging and diverging sections. The maximum detonation velocity also increases as W_{throat}/W_{tube} decreases.

4. Conclusions

This paper presents computationally with the detonation propagating through the converging-diverging nozzles with three throat widths in the mixture of hydrogen/oxygen diluted by argon and nitrogen.

1) When the detonation wave propagates in the converging section, the triple point becomes strong due to the short interval of the collision time with the wall and the shock wave pattern and the detonation velocity is overdriven. High pressure and temperature are observed in the converging section when small W_{throat}/W_{tube} is applied.
2) When the detonation wave propagates in the diverging section, high pressure area remains in the converging section of the nozzle with W_{throat}/W_{tube}= 0.12 for both the argon and nitrogen dilutions.
3) Detonation waves become a deflagration in the case through the nozzle with W_{throat}/W_{tube} = 0.12 for both the argon and nitrogen dilutions. However, the detonation structure is maintained in the nozzle with W_{throat}/W_{tube} = 0.50. The cause of the deflagration in the diverging section comes from that the strong expansion

waves near the throat cut the transverse wave and decrease downstream pressure which is necessary to sustain the detonation wave.

Acknowledgements

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References

[1]Eidelman, S. and Grossman, W., "Pulsed Detonation Engine: Experimental and Theoretical Review," AIAA paper 1992-3168.

[2]Kailasanath, K., "A Review of Research on Pulse Detonation Engine Nozzles," 39th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, AIAA paper 2001-3932.

[3]Yungster, S., "Analysis of Nozzle Effects on Pulse Detonation Engine Performance," 41st Aerospace Science Meeting and Exhibit, AIAA 2003-1316.

[4]Morris,C.I., "Quasi-One-Dimensional Modeling of Pulse Detonation Rocket Engines," 39th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, AIAA 2003-5204.

[5]Edwards, D.H., Hooper, G., and Meddins, R.J., "Instability in the Reaction Zones of Detonation Waves," Astronautica Acta, Vol.17, pp.475-485, 1972.

[6]Petersen, E.L. and Hanson, R.K., "Reduced Kinetics Mechanisms for Ram Accelerator Combustion," *Journal of Propulsion and Power 15* (1999), pp.591-600.

	Ltube [mm]	Lnozzle [mm]	Wtube [mm]
Argon dilution	3.2	1.6	0.4
Nitrogen dilution	8.0	4.0	1.0

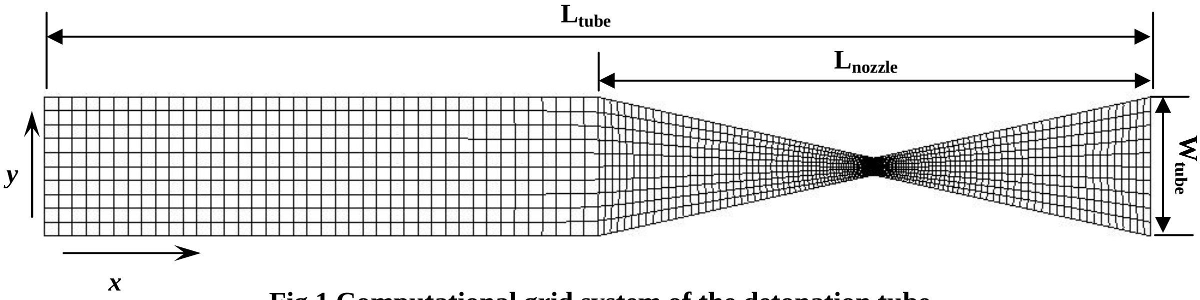
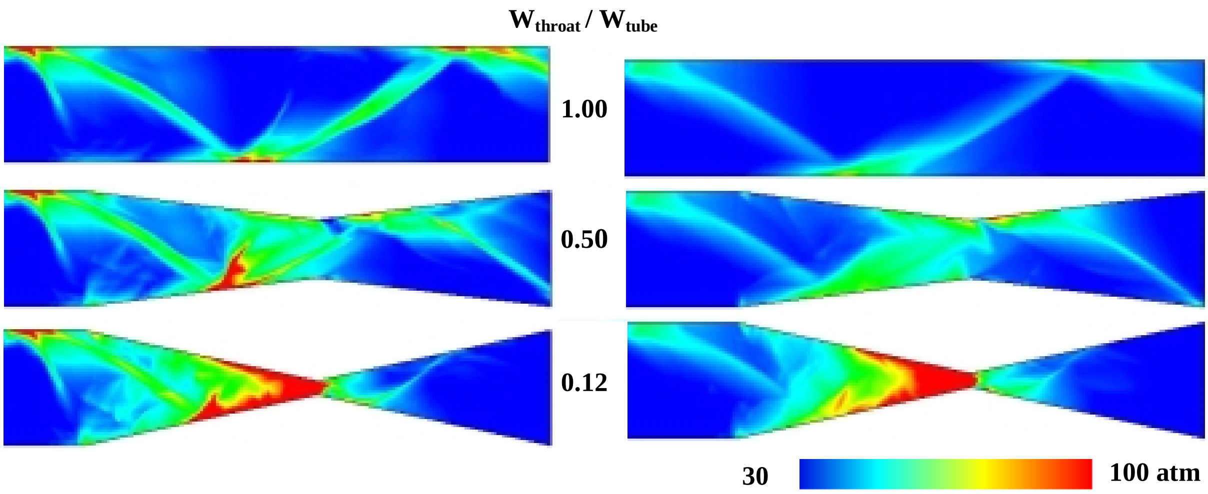
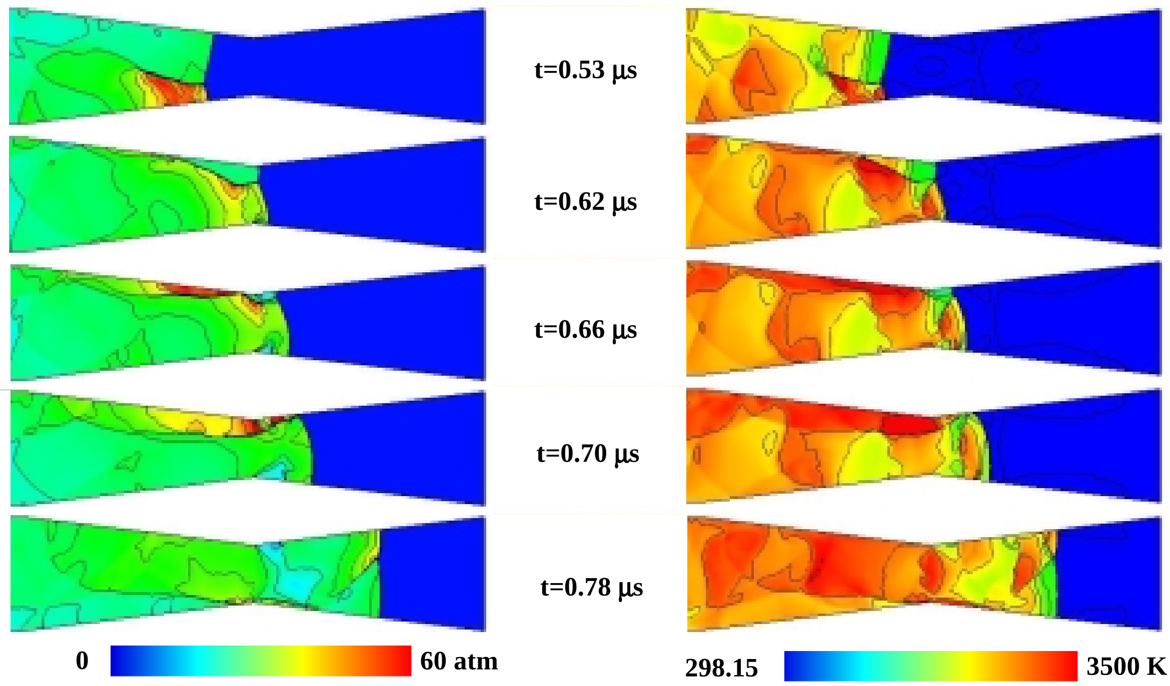


Fig.1 Computational grid system of the detonation tube with a converging-divergent nozzle.



(a) The argon dilution. **(b) The nitrogen dilution.**

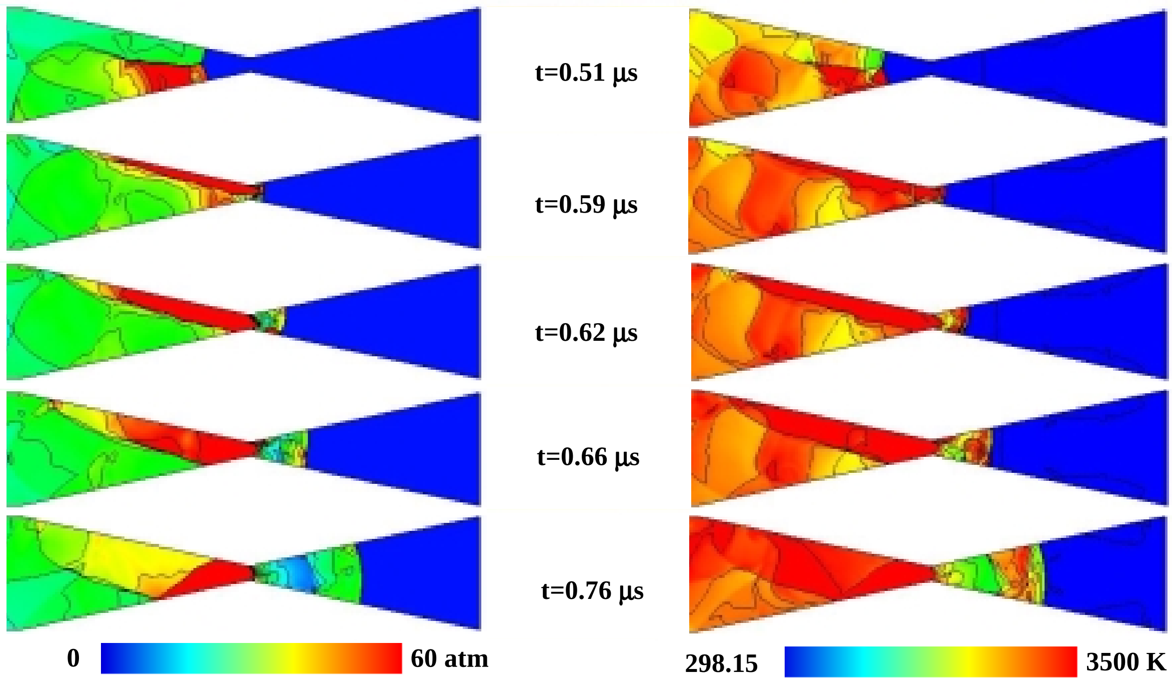
Fig.2 Maximum pressure histories.



(a) Pressure histories.

(b) Temperature histories.

Fig.3 Parameter histories in the case of the argon dilution and the nozzle with W_{throat}/W_{tube}=0.50.



(a) Pressure histories.

(b) Temperature histories.

Fig.4 Parameter histories in the case of the argon dilution and the nozzle with W_{throat}/W_{tube}=0.89.

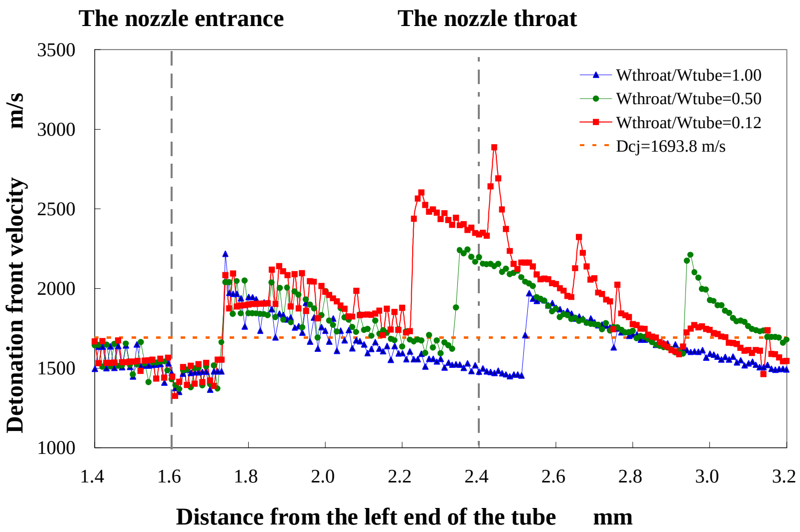


Fig.5 Detonation velocity histories along the nozzle center in the case of the argon dilution.

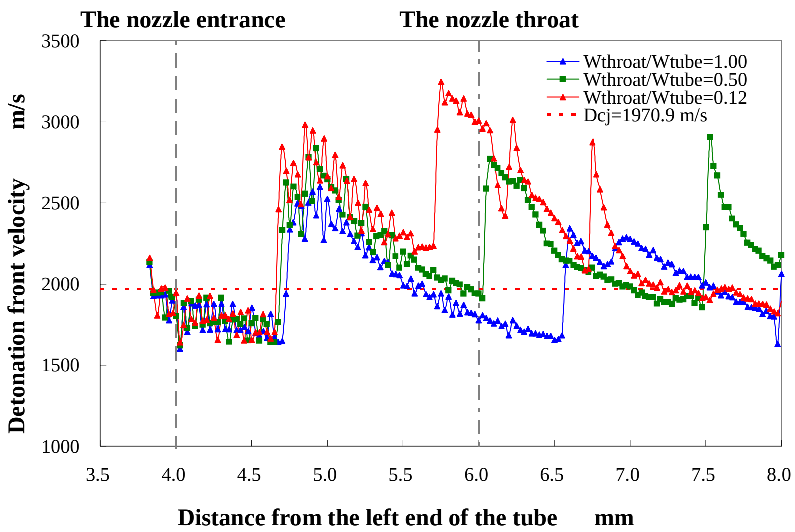


Fig.6 Detonation velocity histories along the nozzle center in the case of the nitrogen dilution.