

Numerical Investigation on Characteristics of a Planar Detonation Wave across Layers of Burned Gas

Naoya OHIRA¹, Akiko MATSUO¹,
Jiro KASAHARA², Ken MATSUOKA²

¹Department of Mechanical Engineering, Keio University,
3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa 223-8522, Japan

²Department of Aerospace Engineering, Nagoya University
Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8603, Japan

1 Introduction

Recently, highly attention has been paid to the development of Rotating Detonation Engines (RDEs) due to their higher thermal efficiency and simpler structure than conventional deflagration engines. RDEs generally have a double-cylindrical chamber which confines detonation waves to keep continuous propagation and generates stable thrust. Fuel-oxidizer reactants enter the chamber through nozzles or slits on the closed end, and burned products exit through the open end. One of difficulties in RDEs is fuel-oxidizer mixing. Due to the operation frequency of kHz order resulting from supersonic detonation waves, incomplete mixing condition appears inside the chamber. In addition, injected reactants are mixed into burned products of previous detonation. Consequently, the interaction between fuel, oxidizer and burned gas would affect the propagation velocity and the stability of detonation waves inside the RDE chamber.

Some experiments about RDEs have reported that propagation velocity of detonation waves was falling below the CJ value. However, the dominant factor in the velocity decrease is still unclear. Fujii *et al.* [1] conducted a two-dimensional numerical simulation to clarify the key factor in the velocity decrease. In their simulation, the distribution of injected reactants and remained products were simplified as striped uniform rectangles. According to their research [1], velocity decreased when the existence of hot burned gas and the non-premixed condition of fuel-oxidizer were observed at the same time, whereas velocity kept approximately the CJ value when either of them was observed.

This research focuses on the effect of burned gas on detonation propagation. To simplify the chamber shape and the non-premixed condition of fuel-oxidizer, the target is a planar detonation wave propagating through the layers of premixed C₂H₄-O₂ gas and burned gas. Both gases have the rectangular shape to simplify injected premixed gas and remained burned gas as well as the work of Fujii *et al.* [1]. Nitrogen is also applied instead of burned gas to clarify the effect of burned gas.

2 Numerical Setup

Figure 1 shows the two-dimensional computational domain, which is composed of the main section and the driver section. The driver section is filled with stoichiometric $\text{C}_2\text{H}_4\text{-O}_2$ mixture. The initial detonation, which is fully-developed in the premixed gas at 1 atm and 293 K, starts to propagate from the right end of this section. Initial values of the CJ velocity $D_{CJ,pre}$, the cell width and the cell length are 2375 m/s, 0.8 mm and 1.4 mm, respectively. There are two initial conditions for the main section described in Fig. 1; (a) inert gas and (b) premixed and burned gases. Rectangles of premixed and burned gas denotes the simplified RDE flow field. Tables 1 and 2 show calculation parameters and characteristics of gases. High temperature burned gas is the main target, and low temperature burned gas and nitrogen are used for comparison. The value of 3500 K is the same as the temperature of detonation products in the work of Fujii *et al.* [1]. 1.6 and 3.2 mm each correspond to shorter and longer value than twice the initial detonation cell length $2L_{pre} = 2.8$ mm. The initial pressure of gases is 1 atm except the initial detonation.

The computational domain is discretized as an orthogonal grid ($\Delta x = \Delta y = 10 \mu\text{m}$) except the stretched region from 5 mm behind the initial detonation front to the right boundary. The top and bottom sides of the domain are adiabatic non-slip walls, the right boundary is the non-reflective boundary proposed by Gamezo *et al.* [2], and the left boundary is located just ahead the leading shock wave and extended leftward with the detonation propagation.

The governing equations are the two-dimensional compressible Navier-Stokes equation for 10 species (C_2H_4 , O_2 , H_2O , CO_2 , H_2 , H , O , OH , CO , N_2). The ideal gas law is utilized to close the equation set and thermodynamic properties are calculated by the NASA polynomials [3]. Yee's non-MUSCL type 2nd-order TVD upwind scheme [4] and the 2nd-order central difference scheme are applied for discretization of convective term and diffusion term, respectively. Chemical reaction model is the detailed reaction model proposed by Singh *et al.* [5] which considers 10 elementary reactions, and the multi-timescale method [6] is chosen as the time integration method for chemical-source term.

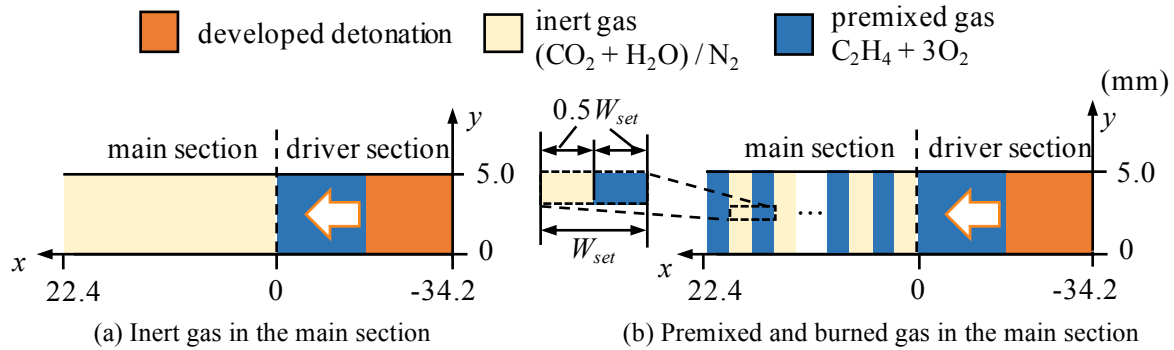


Figure 1. Computational domain and initial condition

Table 1. Calculation parameters

Initial Condition	Inert gas		Set width W_{set} (mm)
	Name	Temp. T_i (K)	
Only inert gas	Burned gas	3500, 1000	—
	Nitrogen	293	
Modeled RDE	Burned gas	3500, 1000	1.6, 3.2
	Nitrogen	293	

Table 2. Characteristics of gases

Name	Component	Temp. (K)	Density (kg/m ³)	Sound speed (m/s)
Premixed	$\text{C}_2\text{H}_4 + 3\text{O}_2$	293	1.29	325
Burned	$\text{H}_2\text{O} + \text{CO}_2$	3500	0.108	976
		1000	0.378	570
Nitrogen	N_2	293	1.17	349

3 Results and Discussion

3.1 Transition from the Detonation Wave to the Shock Wave in Inert Gas in the Main Section

In the inert gas in the main section, the detonation wave changes into a shock wave owing to lack of reactants. Figure 2 shows the propagation velocity histories of the detonation wave or the shock wave on the center line ($y = 2.5$ mm). The blue region in Fig. 2 represents the premixed gas region and the time $t = 0$ μ s corresponds to the time when the leading shock wave reaches the end of the driver section ($x = 0$ mm). Velocity becomes almost steady at $t = 1.0$ μ s in all cases. Table 3 shows velocity and pressure at $x = 20$ mm and $y = 2.5$ mm for all conditions. The value of shock velocity in high temperature burned gas exceeds $D_{CJ,pre}$ by 22% without any reactants, while that in other inert gases are lower than $D_{CJ,pre}$. On the other hand, pressure shows an opposite trend. These differences in velocity and pressure are caused by differences in thermodynamic characteristics such as density, speed of sound and specific heat ratio between each inert gas.

Figure 3 indicates the maximum pressure history at $x = -2.8$ – 2.8 mm. Trajectories of triple points can be seen at the beginning part of the main section ($x = 0$ – 1.4 mm) and gradually disappear at the following part ($x = 1.4$ – 2.8 mm). These trajectories indicate that transverse waves keep own intensity by burning reactants which is advected from the driver section and attenuate when advected reactants are completely consumed. In Fig. 2, velocity peaks appear at the same time ($t = 0.8$ μ s) in all cases. These velocity peaks imply the formation of a Mach stem by the collision of transverse waves. Velocity of transverse waves is probably independent of inert gas characteristics unlike velocity of leading shock waves. Therefore, the cell length at the main section increases as the velocity of leading shock wave becomes higher as shown in Fig. 3.

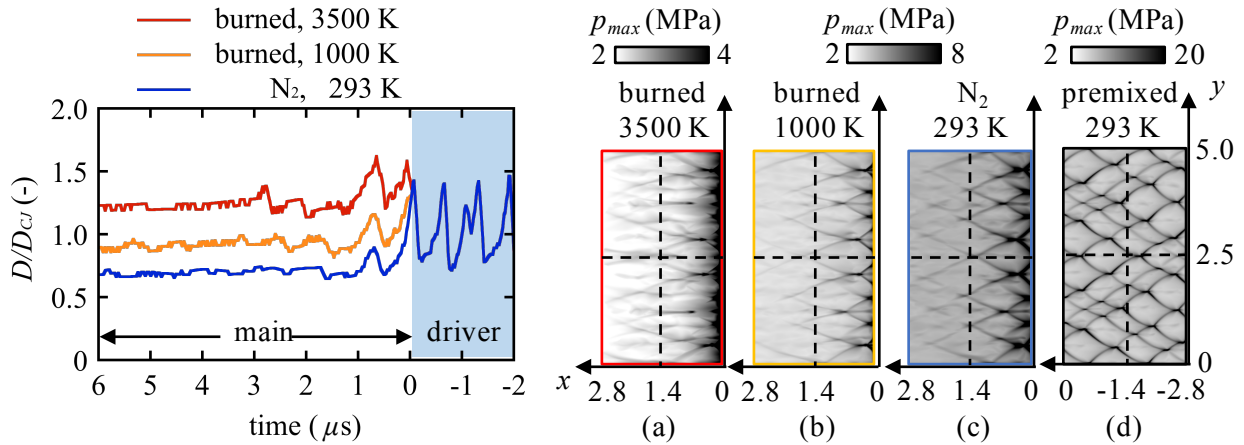


Figure 2. Shock velocity history in only inert gas condition on $y = 2.5$ mm line ($D_{CJ,pre} = 2375$ m/s) (blue: premixed region, white: inert region)

Figure 3. Maximum pressure histories in inert gas (cell length in premixed gas $L_{pre} = 1.4$ mm)

Table 3. Velocity and pressure in inert gas at $x = 20$ mm and $y = 2.5$ mm

Inert gas Name	Temperature T_i (K)	Propagation velocity	Propagation velocity normalized by CJ value	Pressure p (MPa)
		D (m/s)	$D/D_{CJ,pre}$ (-)	
Burned gas	3500	2900	1.22	0.880
	1000	2120	0.895	1.52
Nitrogen	293	1550	0.651	2.44

3.2 Propagation and Decoupling in the Layers of Gases Case

Figure 4 indicates the histories of the propagation velocity on the center line ($y = 2.5$ mm). The periodic velocity oscillation, which is the characteristics of detonation, can be seen in the entire region except the nitrogen case. In the nitrogen case, the propagation velocity once falls, rises up after propagating certain distance, and then shows the periodic oscillation. This behavior indicates that the large decoupling causes at the first layer of nitrogen and the detonation re-initiates later. Table 4 represents each average velocity in the premixed region, the inert region and the whole region at the main section. In all cases, detonation waves are attenuated in comparison with CJ state due to lack of reactants, and the average velocity in the premixed region is lower than $D_{CJ,pre}$. However, the average velocity in the whole region exceeds $D_{CJ,pre}$ in the burned gas of 3500 K cases. Comparing burned gas of 3500 K and 1000 K cases, velocity of the inert region shows large differences. The thermodynamic characteristics of inert gas cause these large differences as mentioned in §3.1. Although the detonation wave is attenuated by the lack of reactants, the average velocity in the whole region keeps $D_{CJ,pre}$ because of high velocity in high temperature burned gas. These results explain the mechanism observed in the work of Fujii *et al.* [1] that the overall propagation velocity maintains approximately $D_{CJ,pre}$ in the RDE chamber including not only premixed gas but also hot burned gas.

Figure 5 indicates the maximum pressure histories in the main section. In burned gas of $W_{set} = 3.2$ mm case, trajectories are highly unstable. This instability represents small decoupling and re-initiation. From Figs. 4 and 5, the detonation wave can propagate continuously in whole region when it reaches the first premixed layer without large decoupling. Therefore, large decoupling occurs when the detonation collapses

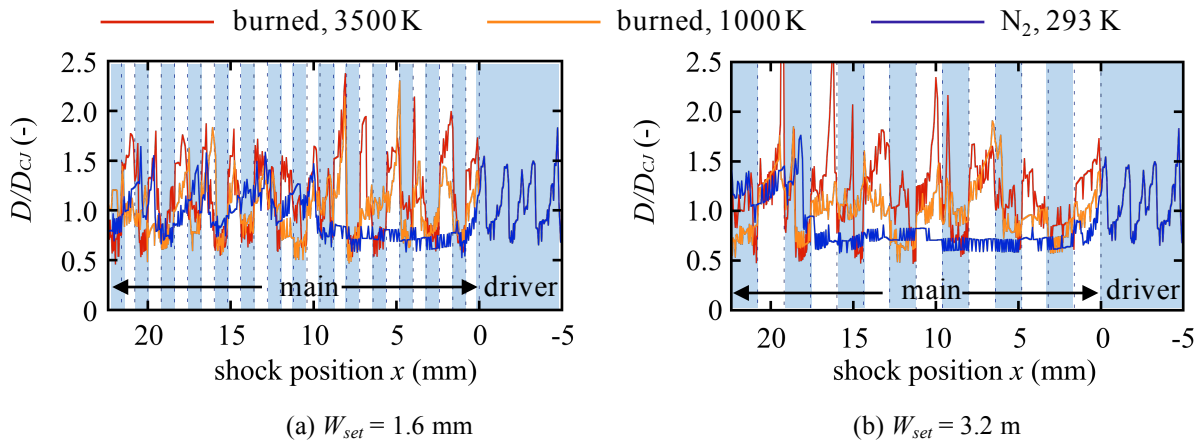


Figure 4. Propagation velocity profiles at $x = -5.0$ – 22.4 mm on $y = 2.5$ mm line
(blue: premixed region, white: inert region, $D_{CJ,pre} = 2375$ m/s)

Table 4. Average propagation velocity in each gas at $x = 0 - 22.4$ mm on $y = 2.5$ mm line

Set width W_{set} (mm)	Inert gas		Average propagation velocity normalized by CJ value $D/D_{CJ,pre}$ (-)		
	Name	Temperature T_i (K)	premixed region	inert region	whole region
1.6	Burned gas	3500	0.823	1.40	1.04
		1000	0.853	1.11	0.963
	Nitrogen	293	0.847	0.908	0.876
3.2	Burned gas	3500	0.886	1.37	1.08
		1000	0.844	1.12	0.961
	Nitrogen	293	0.770	0.786	0.778

in the first layer. Although the detonation restarts in all cases in this research, the rotating detonation wave is hard to re-initiate because there is no support of upper wall in the actual RDE chamber. Therefore, if the width of gap between injection ports exceeds a certain length, the rotating detonation wave probably causes quenching. This length threshold need to be examined in detail.

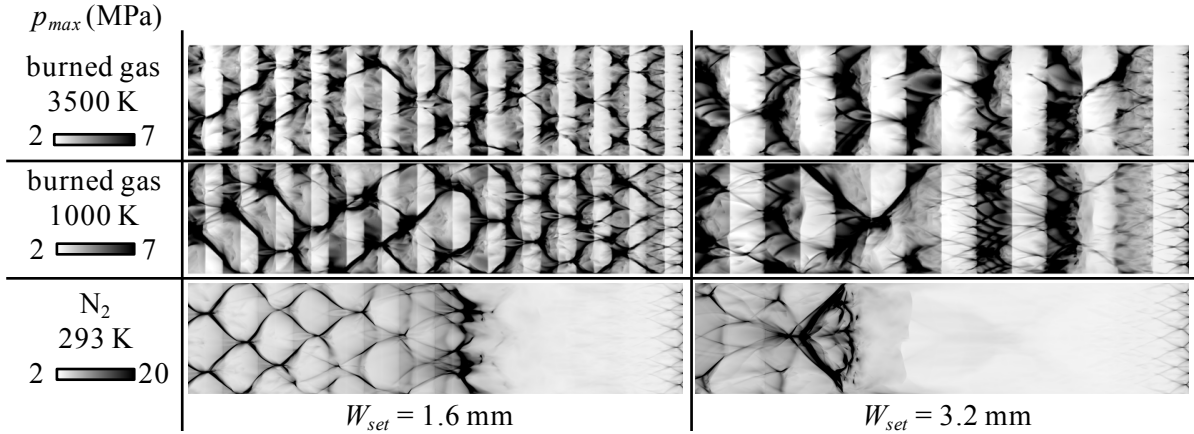


Figure 5. Maximum pressure histories in the main section ($x = 0\text{--}22.4$ mm, $y = 0\text{--}5$ mm)

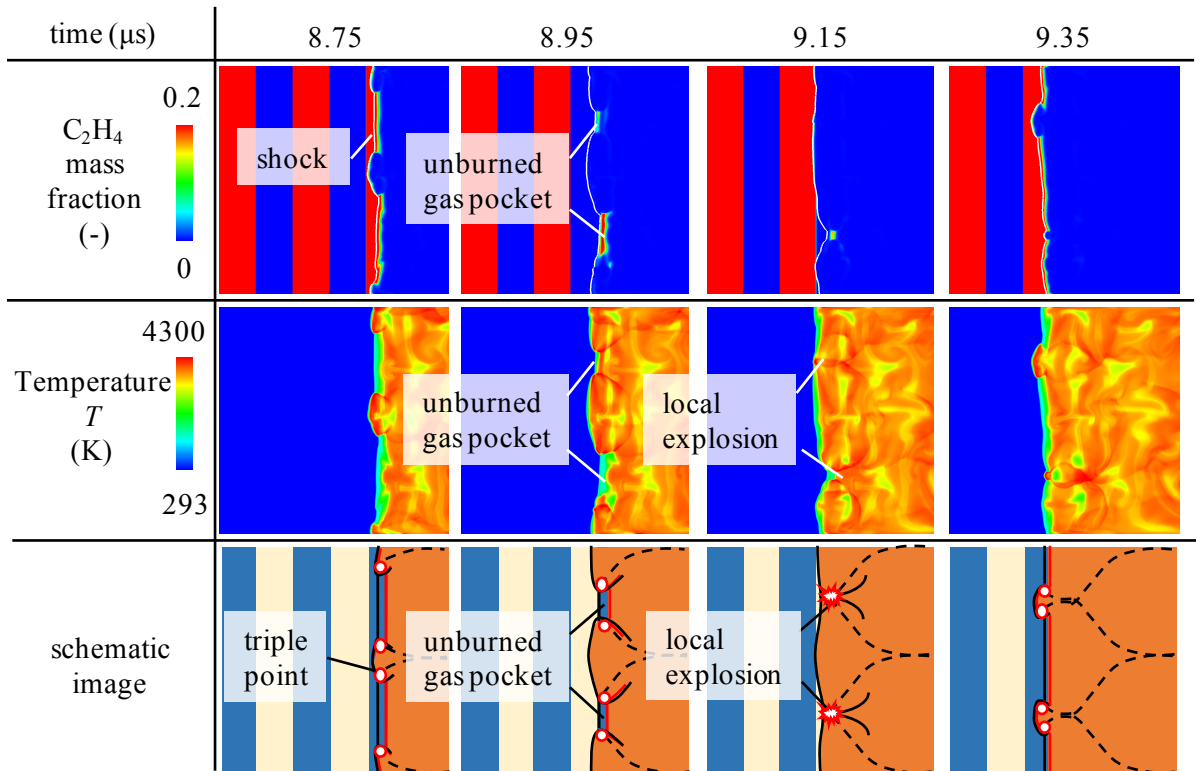


Figure 6. Mechanism of propagation in the layers of gases at $x = 15.8\text{--}20.8$ mm (upper two row: flow field in nitrogen of $W_{set} = 1.6$ mm case, bottom row: schematic image)

The mechanism of continuous propagation across layers of burned gas is shown in Fig. 6. Figures in upper two row illustrate the time sequence of ethylene mass fraction and temperature in nitrogen of $W_{set} = 1.6$ mm case. Figures in bottom row are schematic images. In this case, trajectories of triple points form stable cellular structures after the re-initiation as shown in Fig. 5. When the Mach stem of the detonation front enters the premixed gas region, combustion occurs immediately and new transverse waves are generated. In contrast, ignition delay makes unburned gas behind the weak incident shock wave. This gas is advected to inert gas region, and then the local explosions occur and new Mach stems form when the transverse waves collide. By repeating this mechanism, detonation waves can propagate stably with combustion of unburned gas even in inert gas region. This mechanism that the detonation wave keeps own intensity by local explosion is similar to that in premixed gas.

4 Conclusion

A two-dimensional numerical investigation is conducted to research the effect of burned products that is remained between injected premixed reactants in a RDE chamber. The target is a planar detonation propagating to the flow field containing layers of premixed gas and burned gas/nitrogen. Velocity of the leading shock wave in burned gas is higher than that in nitrogen because of thermodynamic characteristics such as density, speed of sound and specific heat ratio. This is why the average propagation velocity keeps around the CJ value in the RDE chamber which includes not only premixed gas but also high temperature burned gas. In inert gas layer, transverse waves are maintained by the combustion of reactants advected from the premixed gas layer. Therefore, a detonation wave becomes a flat shock wave and causes decoupling when the time to propagate the first layer is long enough to consume the most of reactants.

References

- [1] Fujii J, Kumazawa Y, Matsuo A, Nakagami S, Matusoka K, Kasahara J. (2017). Numerical investigation on detonation velocity in rotating detonation engine chamber. *Proc. Combust. Inst.* 36: 2665
- [2] Gamezo VN, Desbordes D, Oran ES. (1999). Formation and Evolution of Two-dimensional Cellular Detonations. *Combustion and Flame*.116: 154.
- [3] Bonnie JM, Sanford G, Martin AR. (1993). Coefficient for calculating thermodynamic and transport properties of individual species. NASA Technical Memorandum. 4513: 10.
- [4] Yee HC. (1987). Upwind and Symmetric Shock Capturing Schemes. NASA Technical Memorandum. 89464.
- [5] Singh DJ, Jachimowski CJ. (1993). Quasiglobal Reaction Model for Ethylene Combustion. *AIAA Journal*. vol.32, No.1, Technical note: 213.
- [6] Gou X, Sun W, Chen Z, Ju Yu. (2010). A dynamic multi-timescale method for combustion modeling with detailed and reduced chemical kinetic mechanisms. *Combustion and Flame*. 157: 1111.