Detailed Numerical Simulation on Dimethyl Ether/Oxygen Premixture Detonation Using Reduced Chemical Reaction Model - Disturbance of Cellular Structure -

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1 Introduction

Detonation is a phenomenon of self-sustained combustion in premixed gases, which is propagating at supersonic speed. In detonation, the flame propagates while the combustion wave and the shock wave interact with each other. Detonation has a unique propagation structure called a cellular structure. The cell is considered to be the trace of the triple points, which is the intersection of mach stem, incident shock, and transverse wave at the detonation wave front. The shock waves interfere with each other to generate small collisions, which are repeated to form cellular structures. In numerical analysis, the cellular structure can be visualized by plotting the maximum pressure history. The cellular structure is closely related to detonation instability. In general, detonations with disturbed cellular structures are more resistant to flow dilation and obstructions. Therefore, the study of detonation cellular structure is important for both hazard analysis and industrial applications.

Dimethyl ether (DME) has attracted attentions as a new fuel as a new SO_x-free fuel for diesel engines an thermal power generations due to its high cetane number[1]. In literature, there are a few investigations on the detonability of DME. In a numerical study, Mével et al.[2] showed that the detonation of DME/oxygen premixture is not a double cellular structure, but a substructure is observed. Ng et al.[3] studied the detonation of DME/oxygen premixture by experiment using a detonation tube. Reactive Fluid Dynamics Laboratory in Kyushu Institute of Technology has conducted an experimental study of DME-fueled Pulse Detonation Engines[4]. Although DME-fueled detonation has been studied for a long time, there is a lack of numerical analytical studies on disturbance of cellular structure and instability using reduced chemical reaction model.

In this study, the numerical analysis of detonation in DME/oxygen premixture is performed using a reduced chemical reaction model; the detonation propagation characteristics are investigated; and the disturbance of the cellular structure is investigated. Unlike experiments, numerical analysis is characterized by the ability to visualize temperature and pressure contours and to easily calculate local

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values. A two-dimensional unsteady analysis was performed to investigate cellular structure disturbances in DME/oxygen premixture detonation, and a one-dimensional steady analysis is performed to calculate parameters related to cell structure disturbances.

2 Numerical Methods

2-1 1D steady calculation

For the one-dimensional steady-state analysis, the ZND model is calculated using Shepherd's ZND codes[5]. In the ZND model, the detonation wave front is handled as a plane wave, followed by the excitation of the internal degrees of freedom, the radical generation/proliferation phase, and the exothermic reaction phase behind the leading shock wave.

2-2 2D unsteady calculation

The two-dimensional compressible Euler equations are used as the governing equations for the two-dimensional unsteady calculation. The fourth-order accurate TVD Runge-Kutta method[6] is used for the time integral term. The HLLC[7]-LLF[8][9][10] flux is used for the convective term, and the second-order MUSCL method is used for higher-order accuracy. The ERENA[11][12] is used to calculate the source term. The Cantera[13] is used for analysis. The channel length is 66.7cm and the channel width is 1.3cm, respectively.

2-3 Initial condition

The common initial conditions, a temperature of 298K, a pressure of 0.1 atm, and stoichiometric ratio, are used for all analyzes performed in this study.

2-4 Chemical reaction model

In this study, the reduced model by Zhao et al.[14] is used as a detailed chemical reaction model. This reaction model is created by Williams et al. There are 55 chemical species and 290 elementary reactions. This reduced model is applicable to a wide range of temperature.

3 Results and Discussion

3-1 1D Calculation Results

Figure 3.1.1 shows the ZND results of temperature and pressure, and Fig. 3.1.2 shows the ZND result of thermicity (1/s). Thermicity is an indicator of the degree of energy release. The left end is the detonation front, and the horizontal axis is the distance from the detonation front. In Fig.3.1.1, the temperature increases and the pressure decreases behind the detonation front, however, their gradient is not a constant value in the reaction region. In Fig. 3.1.2, a two-stage energy release characteristic of DME detonation is seen.

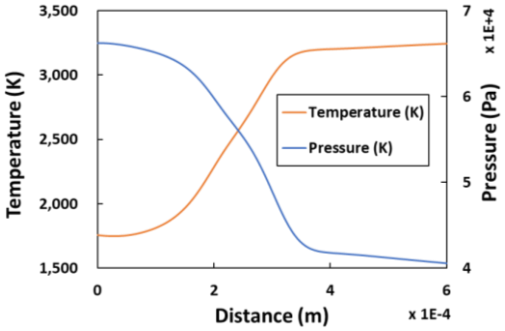

Fig. 3.1.1 Temperature and pressure profiles.

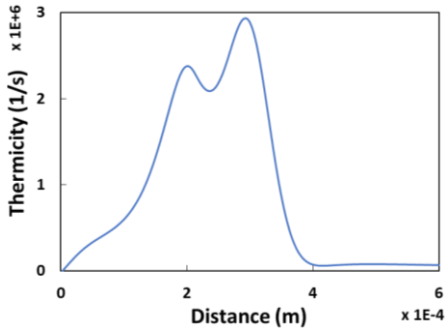

Fig. 3.1.2 Thermicity.

Equation (3.1) [15] is the definition of the reduced activation energy (θ). The reduced activation energy is a quantity that indicates the relative sensitivity of the reaction rate to temperature changes at the temperature behind the shock wave, T_{VN}. E_a is the activation energy; R is the gas constant; τ_1 and τ_2 are induction time; T_1 and T_2 are temperature behind the shock wave, and their suffixes 1 and 2 represent the points of ±1% of the CJ velocity, respectively.

$$\theta = \frac{E_a}{RT_{VN}} = \frac{1}{T_{VN}} \frac{ln\tau_2 - ln\tau_1}{\frac{1}{T_2} - \frac{1}{T_1}} \qquad (3.1)$$

The calculated reduced activation energy in this condition is θ ≈ 10. Next, the stability parameter (χ) is defined in Eq. (3.2). Δ_i is induction length; Δ_R is reaction length; σ_{max} is maximum value of thermicity, and u_{CJ} is CJ velocity, respectively.

$$\chi = \theta \frac{\Delta_i}{\Delta_R} = \theta \Delta_i \frac{\sigma_{max}}{u_{CJ}} \qquad (3.2)$$

In the present conditions, the calculated instability parameter becomes χ ≈ 7.3.

In general, the propagation velocity of the head shock wave varies from 0.85 to 1.2 times the CJ velocity inside the cell[16]. θ in Eq. (3.2) varies within the range of 7 < θ < 14 inside the cell. This makes the induction length approximately 23 times larger inside the cell. It is considered that the cellular structure is greatly disturbed when the variation of the induction length due to the variation of the detonation speed becomes several tens of times. A study by Ng et al.[17] estimated that detonation propagation is stable at χ ≈ 1.5. Therefore, the detonation propagates unstably because of χ ≈ 7.3 under the conditions of this time.

3-2 2D Calculation Results and Cell Structure

In the 2D analysis, the causes of cellular structure disturbance are investigated from two perspectives: transverse detonation and sub-structure. Figure 3.2.1 shows the local maximum pressure history. The cellular structure is very irregular.

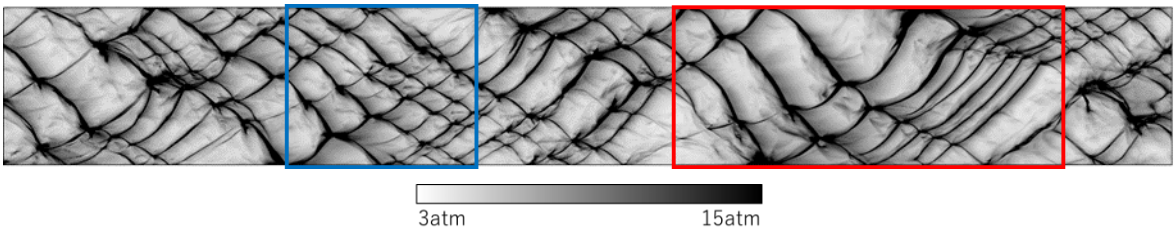

Fig. 3.2.1 Maximum pressure history (Detonation propagates from left to right).

3-2-1 Cellular bifurcation by transverse detonation

Figure 3.2.2 shows an image extracted from the red frame part of Fig. 3.2.1. It can be seen that the large cells are branched into small cells. Figures 3.2.3 and 3.2.4 show the instantaneous temperature and pressure contour. They change from (1) → (2) → (3) → (4). The red lines and numbers in Fig. 3.2.2 indicate the rough positions of the detonation fronts in Figs. 3.2.3 and 3.2.4, respectively. Referring to the study by Asahara et al.[18], Figs. 3.2.3 and 3.2.4 show that the compression wave is advancing toward the unburned gas pocket in Scene 1. In scene 2, a local detonation occurred on the lower wall and a transverse detonation occurred. In Scene 3, the transverse detonation advances toward the upper wall while burning unburned gas. In scene 4, the compression wave generated from behind the transverse detonation propagates to the Mach stem as a disturbance and generates a new transverse wave. This is thought to cause cell branching.

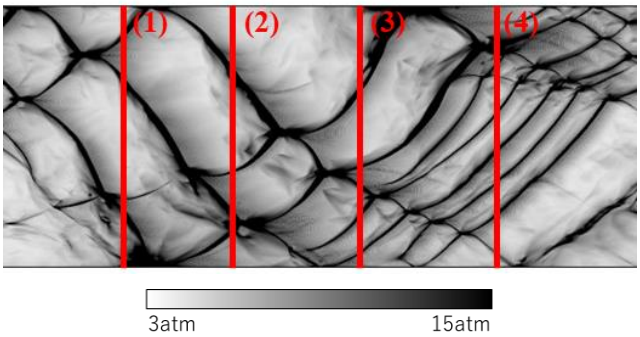

Fig. 3.2.2 Maximum pressure history (extracted from the red frame part of Fig. 3.2.1).

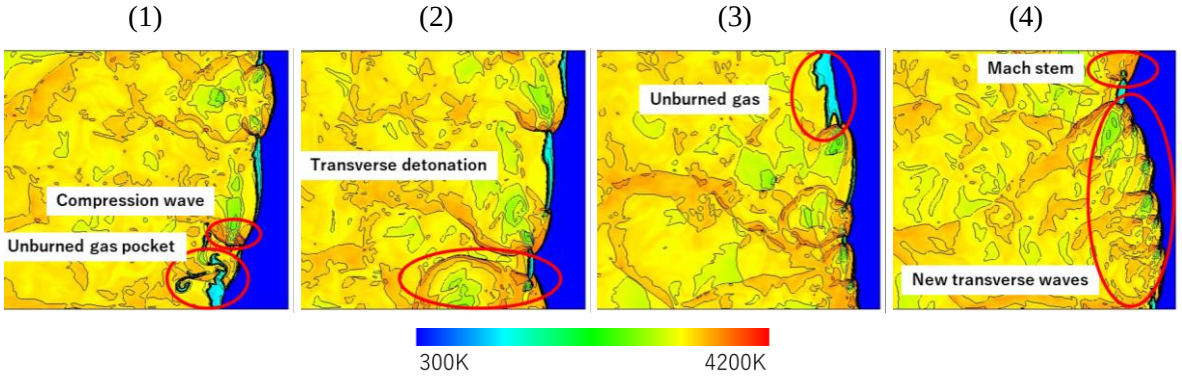

Fig. 3.2.3 Instantaneous temperature profiles ((1) → (2) → (3) → (4)).

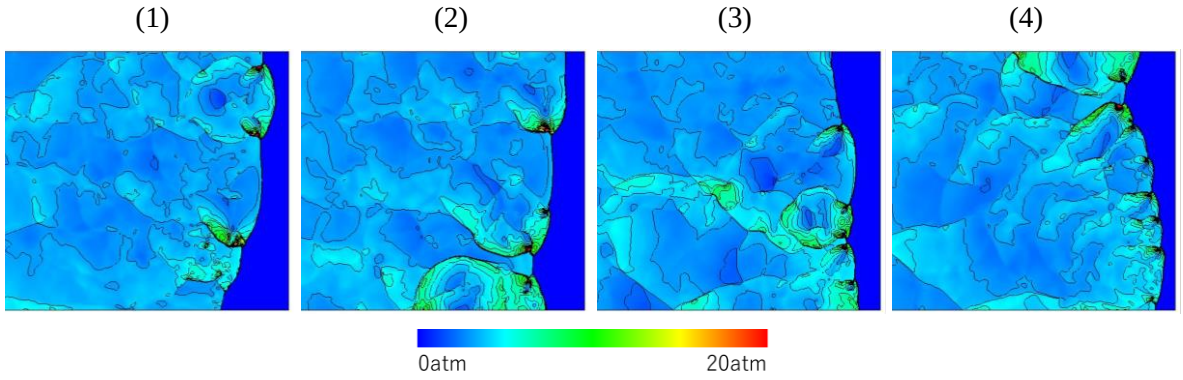

Fig. 3.2.4 Instantaneous pressure profiles ((1) → (2) → (3) → (4)).

3-2-2 Cellular bifurcation by sub-structure

Figure 3.2.5 shows an image extracted from the blue frame part in Fig. 3.2.1. Figure 3.2.6 shows the instantaneous temperature and pressure contours when the detonation front comes roughly to the red line in Fig. 3.2.5. Figure 3.2.5 shows that the weak wave disturbs other cells and divides into the cells. Ng et al.[2] reported that double cells were observed in the experiment at φ=1 below 5 kPa. Mével et al.[1] also did that sub-structures were observed at 5 kPa with equivalent ratios of 0.5 and 1.5 in the numerical analysis. The sub-structure is a weak wave inside the cell. In the present study, no clear sub-structure was observed, but weak waves as shown in Figure 3.2.5 were observed within many cells, which was observed to be one of the causes of cell splitting and disorder. These weak waves are considered to be sub-structures that failed to grow.

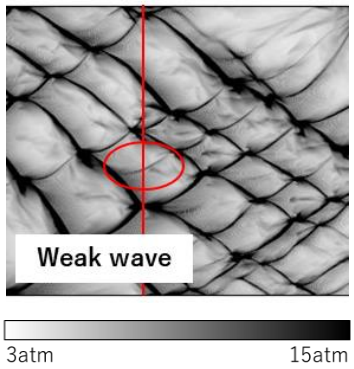

Fig. 3.2.5 Maximum pressure history (extracted from the blue frame part of Fig. 3.2.1).

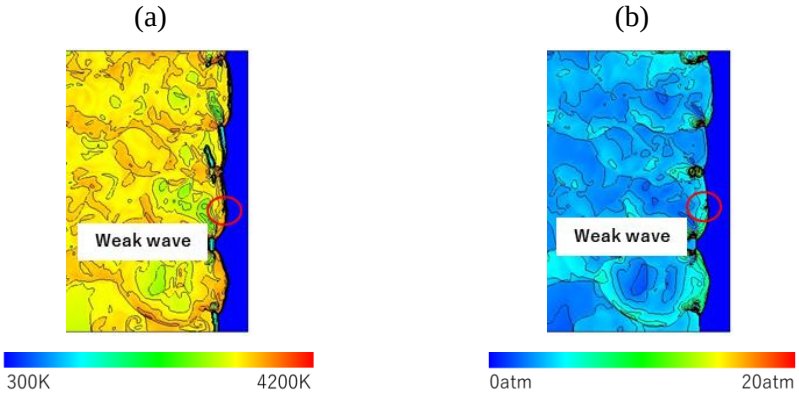

Fig. 3.2.6 (a) Instantaneous temperature profile and (b) Instantaneous pressure profile.

5 Conclusions

· In the ZND analysis, a two-step peak of thermicity is observed.
· The present results show the relative high reduced activation energy and stability parameter.
· In consideration of cell structure disturbance, the cell bifurcation due to the transverse detonation, a large change in induction length inside the cell, and the cell bifurcation due to weak waves are observed.

Acknowledgments

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