

Two-dimensional Numerical Simulations on Unstable Propagation of Propane/Oxygen Detonation Using a Detailed Chemical Mechanism

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1 Introduction

Detonation is a supersonic combustion phenomenon where high-pressure and high-temperature reactions are involved. If detonation happens in factories or power plants, it is presumed that they will suffer serious damages. In fact, some explosion accidents involved with detonation have been confirmed all over the world [1] [2]. Therefore, from the viewpoint of the safety engineering, research on detonation starting conditions and detonation propagation limit, etc. is very important.

Research on unstable detonation propagation is one of the most important research among basic detonation research. Austin et al. [3] investigated on the wave front structure of the unstable detonation in detail using Schlieren and planar laser induced fluorescence techniques. In numerical analysis, Gamezo et al. [4] performed numerical simulations of cellular detonations with different activation energies. They also investigated the numerical noise effect on the cellular structure and concluded that the detonation cell size and cellular structure regularity are not affected by the numerical noise. In addition to these studies, to clarify the effect of diffusion in detonation structure, two-dimensional numerical simulations are performed by Radulescu et al. [5] [6]. They reported diffusion has a significant influence on the reaction of the gases passing across the detonation front in unstable cellular detonation. Gamezo et al. [4] and Radulescu et al. [5] [6] used the single step Arrhenius model as a reaction mechanism. In this study, we use a detailed

chemical mechanism as one possible mechanism to capture the correct sensitivity to a range of temperatures and obtain the correct induction/reaction length.

Our final goal of this study is to clarify the cause of cell size inhomogeneity and velocity oscillation of propane/oxygen detonation, which is considered to be more unstable than hydrogen/oxygen detonation and highly diluted detonations. As the first step, we perform two-dimensional analysis and investigated the propagation behavior of unstable propane/oxygen detonation for different channel width using a detailed chemical kinetic mechanism.

2 Numerical Methods and Conditions

2.1 Numerical methods

In this study, the governing equations are the two-dimensional compressible Euler equations since the influence of viscosity is small in the vicinity of the detonation wave front. UC San Diego mechanism [7], which includes 57 species and 268 elementary reactions, is used for the chemical reaction mechanism for reliability in simulations of high temperature ignition and detonations. The time integration method uses 10 steps 4th-order Total Variation Diminishing Runge-Kutta method (TVDRK) [8]. Advection Upstream Splitting Method flux Difference and flux Vector scheme (AUSMDV) [9] with 2nd-order MUSCL and minmod limiter is used for the numerical flux in the convective term. The chemical reaction source term is integrated by the Extended Robustness-Enhanced Numerical Algorithm (ERENA) [10], which is a stiff solver for a strong stiffness in the complex reaction system.

2.2 Numerical conditions

Figure 1 shows the calculation domain of the present study. In order to reduce the calculation cost, the shock wave coordinate system is used. The boundary condition on top and bottom walls is slip and adiabatic wall condition. Outlet condition is decided by referring to the conditions of Gamezo et al [4]. Y_b , Y_1 , and Y_e mean every boundary value, the current value in the first cell near the boundary, and the extrapolation limit, respectively. The unburned gas is composed of stoichiometric propane/oxygen premixed gas at 0.1 atm and 298.15K. A small portion of unburned gas is placed behind the shock wave as a disturbance to start detonation and otherwise enters with Chapman-Jouguet (CJ) detonation velocity from the inlet side. The One-dimensional numerical result is also used for igniting the detonation.

The detonation Induction length was determined to be 390 μm , which is calculated by Zel'dovich-von Neumann-Döring (ZND) model. Table 1 shows the calculation cases of this study. The simulations were performed for two different channel widths. The grids are 3 μm orthogonal grids, which means that 130 grid points are contained in the induction length.

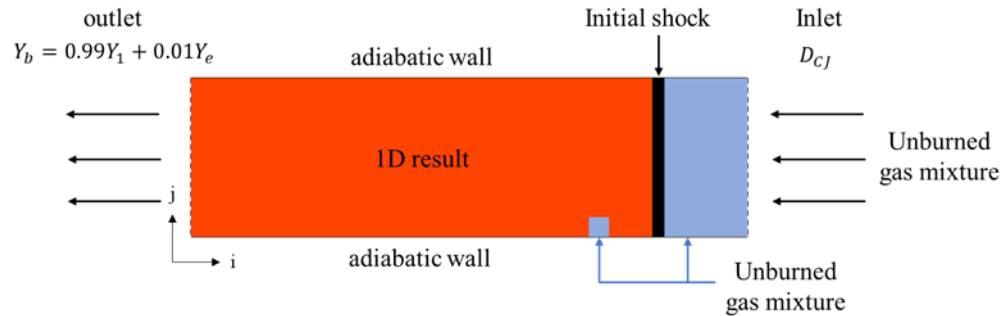


Figure 1. Schematic of the calculation area.

Table 1. Calculation conditions

	Channel width d [mm]	Grid width [μm]	Grid points
Case 1	1.5	3	2501 x 501
Case 2	3.0	3	5001 x 1001

3 Results and Discussions

3.1 The effect of channel width

Figure 2 shows the pressure and density gradient distribution of the detonation wave front. The propagation direction is left to right. From the pressure distribution in Case 1, the Mach stem (MS), the incident shock wave (IS), the transverse wave (TW), and the triple point (TP) can be confirmed. In Case 1, the detonation wave propagates while having a single triple point, whereas it propagates while having two triple points in Case 2. Furthermore, we investigated the detonation propagation mode by looking at the maximum pressure histories which correspond to soot foil records in experiments. From Fig. 3(a), Case 1 shows single-headed mode and its cell length a constant value. In this case, the pressure is very high in the vicinity of the wall surface. Therefore, it is conceivable that detonation wave propagates while repeating explosions near the wall surface. The same result has been reported in the ethylene/oxygen detonations with multi-stepped chemical reaction mechanism [11]. In contrast, Fig. 3(b) for Case 2 shows a very complicated pressure history, indicating that it is not a single-headed mode but a multi-headed mode. Unlike Case 1, Case 2 has various detonation cell sizes from as much as channel width to a very small one. It is thought that this is due to the irregular occurrence of detonation at various places besides walls. As a result, cellular instability was observed in Case 2, but not in a narrow channel (Case 1). Therefore, when the channel width is too narrow, instability of detonation cannot be seen (in this case at least 3 mm seems to be the needed channel width). The cell width obtained in the experiment under this condition is about 10 mm, which is approximately three times the cell width obtained in Case 2. This is considered to be due to the fact that the number of initiations has increased more than in experiments because energy is evaluated without considering the depth direction in two-dimensional calculations.

Figure 4 shows the velocity histories at the center line of the channel. The vertical axis is non-dimensional by dividing the detonation wave velocity by the CJ detonation velocity. In Case 1, it is clear that the detonation wave propagates with an amplitude of about $1.5 D_{CJ}$ except for one place. The amplitude rapidly increased around 108 mm because the local explosion happens at that point. It is confirmed that the detonation wave attenuates from around 125 mm to near the CJ velocity and finally disappears. As for Case 2, it is clear that detonation is propagated at about 5mm wavelength around 90 – 102 mm where the cell width is equal to the channel width. After that, as the cell width becomes irregular, the detonation wave propagates with various velocity amplitudes.

3.2 Distribution of chemical species

Figure 5 shows the Instantaneous temperature and chemical species distribution near the detonation wave front in Case 2. As representative chemical species in propane/oxygen detonation, the distribution of hydroxy group, hydrogen peroxide, normal propyl group, and isopropyl group are shown. From line (a) distributions, we can know the Induction length behind the Incident shock. It is about $210 \mu\text{m}$ and about half of Δ_{ZND} , which is the length obtained by the ZND model. Similarly, for the line (b), the induction length behind the Mach stem is $8 \mu\text{m}$ small, which is only 2% of Δ_{ZND} . Focusing on the change in mass fraction, it can be seen that mass fraction rises gently behind the Incident shock, however, behind the Mach stem, it sharply rises after adiabatic compression and heating by the shock wave.

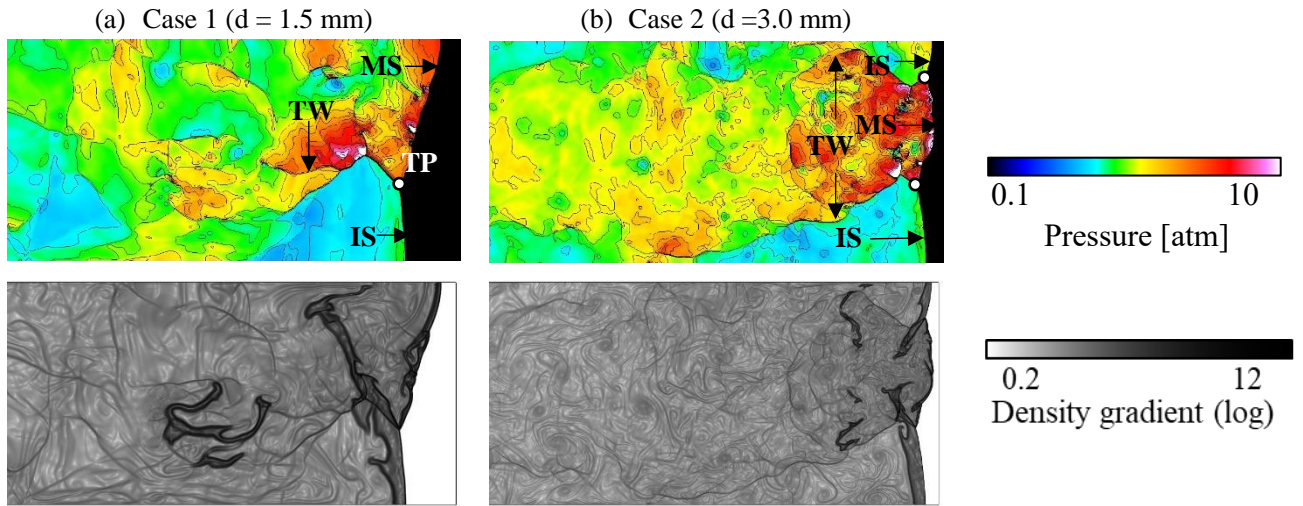


Figure 2. Instantaneous pressure and density gradient contours.

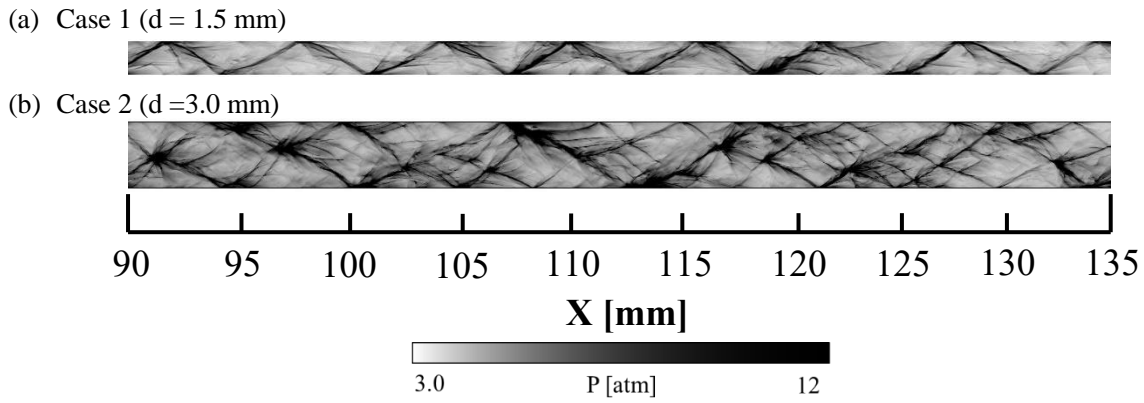


Figure 3. Comparison of maximum pressure histories.

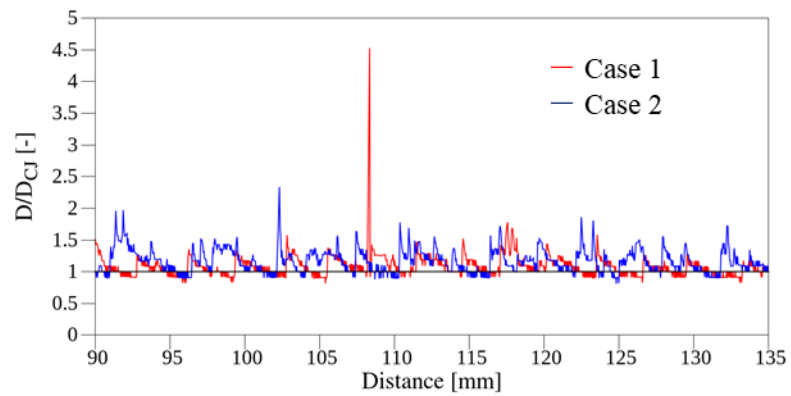


Figure 4. Comparison of velocity histories.

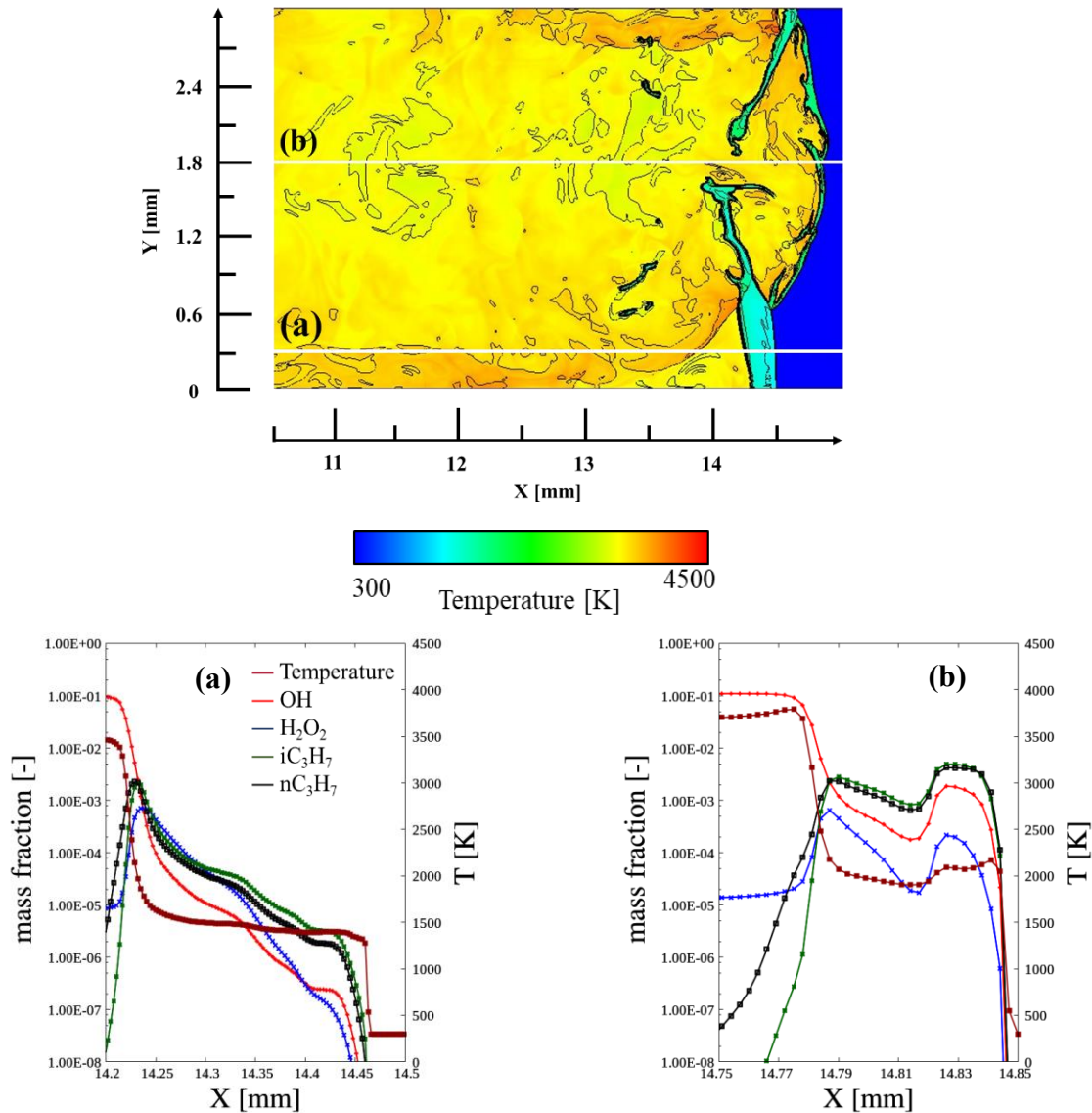


Figure 5. Instantaneous temperature and chemical species distribution along with line (a) and (b).

(White lines indicates (a) $Y = 0.3$ mm, (b) $Y = 1.8$ mm, respectively.)

4 Conclusions

Two-dimensional detonation simulations in the premixed propane/oxygen gas with detailed chemical reaction mechanism for different channel width are performed to conclude as follows:

- (1) When the channel width is 1.5 mm, the detonation propagation mode is single-headed-mode, and detonation propagates with a single triple point while reflecting on the upper and lower surfaces.

- (2) When the channel width is 3.0 mm, there are two triple points, and the triple points propagate while interfering with each other besides the upper and lower surfaces of the channel.
- (3) The cell size obtained by present works is 3.0 mm at maximum, which is about one third of the cell size obtained from the experiment under the conditions.
- (4) From the maximum pressure history and the velocity history, it was found that detonation with strong instability is more likely to propagate.
- (5) The chemical reaction occurred rapidly behind the Mach stem, and its induction length was about 2% of Δ_{ZND} .

Acknowledgments

This research has collaborated with the Research Institute for Information Technology, Kyushu University.

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