# Two-dimensional Numerical Analysis on Shock Flame Interaction in Premixed Gas of Hydrocarbon/Oxygen with Multi-step Reaction Model

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### 1 Introduction

Detonation is a combustion phenomenon propagating with shock waves and has some characteristics, for example hypersonic, high pressure and high temperature. These characteristics cause serious damage when detonation occurs, so in terms of safety engineering, it is very important to research the initiation of the detonation. There are mainly two types to initiate the detonation :direct initiation and indirect initiation. The indirect initiation is also called Deflagration-to-Detonation Transition(DDT), and its process is generally separated into two processes. One is the flame acceleration process and the other is the process that local explosions cause detonation. Shock/flame interaction is one of the reasons why flames are accelerated and has been investigated experimentally [1, 2] and numerically [3-5] for about 50 years after starting with the work of Markstein[6]. Two-dimensional [3] and three-dimensional [4] numerical simulations on the SFI in ethylene/air premixed gas were performed by Gamezo et al. using the one-step reaction model. The object in these researches is the phenomenon that the flame interacts with the shock wave immediately after the start of calculation. Therefore, it is possible to apply the one-step reaction model, which is generally thought to be unable to capture the flame propagation [7-9]. On the other hand, Matsumoto et al. carried out the experiments about the SFI in methane/oxygen/nitrogen premixed gas [1] that the flame interacts with the shock after the flame propagates along some distance. The final goal of our research is to simulate in the same experimental conditions by Matsumoto et.al [1] and compare the numerical simulation with the experiments. We have been carrying out the SFI simulations using the multi-step reaction model, which can capture the flame propagation more accurately than the one-step reaction model.

The objective of this paper is to investigate the grid resolution and the qualitative effect of the incident shock Mach number on the shock/flame interaction in hydrocarbon premixed gas. As a preliminary step for

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the final goal, we simulate the shock/flame interaction in ethylene/oxygen premixed gas, which is relatively lower computational cost than methane/oxygen premixed gas.

### 2 Numerical method and conditions

#### 2.1 Numerical method

The Euler equations are usually adopted when the detonation simulation is performed. This is because detonation is a hypersonic phenomenon so the effects of transport phenomena, such as the diffusion, heat conduction, and viscosity are to be negligible. However, the effects of the boundary layer are important in DDT. Therefore, we solve the Navier-Stokes equations for a system containing premixed ethylene and oxygen gas mixture. The reaction of ethylene/oxygen is reproduced by the multi-step model including 23 species and 38 elementary reactions [10]. The governing equations are explicitly integrated using 3rd-order Total Variation Diminishing Runge-Kutta method [11]. The chemical reaction source term is integrated the Extended Robustness-Enhanced Numerical Algorithm [12], which is the stiff solver for complex chemical reaction system to avoid a stiff problem. Advection Upstream Splitting Method flux Difference and flux Vector scheme(AUSMDV) [13] with 2nd-order Monotone Upstream-centered Scheme for Conservation Laws [14] and minmod-limiter is used for the numerical flux in the convective term. The discretization of the viscosity term is evaluated by the 2nd-order central difference.

### 2.2 Numerical conditions

Figure 1 shows the computational setup of the present study. In order to reduce computational cost, the half of entire domain is adopted. The adiabatic flame calculated under 0.1 atm and 298.15 K by AISTAJAN [15] is pasted near the left wall. The shock in the right of computational domain uses the result of one-dimensional shock tube simulation. The ambient region is filled with stoichiometric ethylene/oxygen premixed gas. These conditions are that the pressure is 0.1 atm and the temperature is 298.15 K, respectively. Maximum Courant-Friedrichs-Lewy number sets 0.4.

Table 1 shows the summary of the grid systems. Both of two grid types use small grid width near the wall to capture the boundary layer. By combining the grid resolution and the incident shock's Mach number  $M_s$ , we selected the three cases, Case 1, Case 2 and Case 3 in Tab. 2.



Figure 1. Schematic of the computational setup.

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	Grid points	$\Delta x$	$\Delta y_{min}$	$\Delta y_{max}$
Coarse	1601 x 101	30µm	10µm	50µm
Fine	3201 x 201	15µm	10µm	25µm

Table 2. Calculation cases.

	Grid	M <sub>s</sub>
Case 1	Coarse	1.97
Case 2	Fine	1.97
Case 3	Coarse	1.61

## 3 Results and discussions

## 3.1 The effects of grid resolution (Case 1 vs Case 2)

Figure 2 is the instantaneous contours of temperature. The flame is compressed by the incident shock in Fig. 2(a), after that, in Fig. 2(b), the flame and the bifurcated shock propagate toward right direction. In Fig. 2, we compare the coarse grid with the fine grid when the contact point between the bifurcated shock and the lower wall comes to the same position. Firstly, there is no large difference on the shape of the bifurcated shock and the flame in Fig. 2(a). That is to say, the effect of grid resolution does not have a large impact shortly after the interaction. On the other hand, in Fig. 2(b), the bifurcated shock shape and the rough flame shape in the coarse grid agree with ones in the fine grid. However, the combustion speed in the coarse grid is faster than that in the fine grid, and the upper flame (flame along the symmetry wall) propagates farther than that in the fine grid. Moreover, there are less unburned gas region between the upper flame and the lower flame (flame along the lower wall) in the coarse grid. Therefore, the bifurcated shock can be analyzed in the coarse grid but the analysis on the flame requires more grid resolution.

In terms of the number of local explosion, there is a difference between the coarse and the fine. In the coarse grid, the local explosion occurs twice, but in the fine grid, local explosion is only once. In Fig. 3(a) shows the instantaneous contours of temperature and the profile along the white line on the temperature contour just before the second explosion in the coarse grid. The local explosion occurs in the yellow circle. On the other hand, the contact point between the bifurcated shock and the lower wall in Fig. 3(b) is the same as that in Fig. 3(a). We compare the yellow circle in Fig. 3(a) (local explosion occurs) to the broken yellow circle in Fig. 3(b) (local explosion does not occur). Regarding the temperature, both Figs. 3(a) and 3(b) are 1300 – 1500 K and there is no large difference. However, pressure in Fig. 3(a) is more than 20 atm whereas one in Fig. 3(b) is only about 5 atm. The difference on pressure between them may have an impact on the occurrence of the local explosions.

## 3.2 The effects of M<sub>s</sub> (Case 1 vs Case 3)

Figure 4 shows the instantaneous contours of density gradients when the flame interacts with the incident shock. Figure 4(a) is the flow field for  $M_s = 1.97$  and Figure 4(b) is that for  $M_s = 1.61$ , respectively. The letters in this figure indicate the flame (**F**), the incident shock (**IS**), the reflected shock (**RS**), the recirculation area (**R**), the bifurcated shock (**BS**), and the upper flame (**UF**). The interaction produces many shocks and they reflected on the walls. These phenomena can be observed for both cases. However, their flame shapes are different. For  $M_s = 1.97$ , the flame after the interaction is divided into upper and lower regions, and both of them propagate toward right. Moreover, the lower flame **R** attaches to **BS** at the bottom wall on this case. On the other hand, the flame for  $M_s = 1.61$  is also divided into two regions but both of them do not propagate toward right. In the high Mach number case, the velocity behind the reflected shock is fast so **UF** and **R** can develop to right. However, in the low Mach number case, the velocity behind the reflected shock is slow so **UF** is involved in **R** behind **BS** and cannot propagate toward right.



ter the reflection. (b) After the propagation to some extent. Figure 2. Flame propagation after the reflection.

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Two-dimensional Navier-Stokes simulations in the premixed hydrocarbon/oxygen gas with the multi-step reaction model for the shock/flame interaction are performed to conclude as follows:

- (1) The grid resolution does not have a large impact on the flame and the bifurcated shock just after the reflection; however, when the flame and the shock propagate to some extent, the combustion speed in the coarse grid is faster than that of in the fine grid.
- (2) Even if the temperature is about the same, no local explosions occur unless the pressure is high.
- (3) The flame after the interaction is divided into two regions and the reflected shock and the bifurcated shock appear. The upper flame develops for the high shock Mach number case ( $M_s = 1.97$ ); however, the upper flame does not propagate for the low shock Mach number case ( $M_s = 1.61$ ).

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Figure 3. Instantaneous contours of temperature and profiles just before the second local explosion.



Figure 4. Instantaneous contours of density gradients after the interaction in Cases1 and 3.