NUMERICAL INVESTIGATION OF DETONATION IN STRATIFIED COMBUSTIBLE MIXTURE AND OXIDIZER WITH CONCENTRATION GRADIENTS

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ABSTRACT

Hydrogen leakage in a closed space is one of the causes of serious accidents because of its high detonability. Assuming the situation that hydrogen is accumulated in a closed space, two-dimensional numerical simulation for hydrogen oxygen detonation which propagates in stratified fuel and oxidizer with concentration gradient is conducted by using detailed chemical reaction model. The concentration gradient between fuel and oxidizer is expressed by changing the number of hydrogen moles by using sigmoid function. Strength of discontinuity at the boundary is controlled by changing the gain of the function. The maximum pressure history shows that the behavior of triple points is different depending on the strength of discontinuity between the two kind of gas. In without concentration gradient case, the transverse waves are reflected at the boundary because of the sudden change of acoustic impedance ratio between two kind of gas. In contrast, in with concentration gradient case, the transverse wavs are not reflected in the buffer zone and they are flowed into the oxidizer as its structures are kept. As a result, the confined effect declines as the strength of discontinuity between the two kind of gas is weakened and the propagating distance of detonation changes.

1.0 INTRODUCTION

Detonation is one of the premixed combustions induced by shock waves. The pressure and temperature of burned gas after the detonation is higher than those after the deflagration. When detonation occurs accidentally, not only the building, but surroundings may be damaged seriously. Considering hydrogen leakage in a building as one accidental situation, hydrogen is mixed with air and accumulated around the ceiling because of the difference of density. In other word, the layer of combustible mixture is produced between a rigid wall and air. Therefore, to know the characteristics of detonation in stratified combustible mixture and oxidizer is important in the practical point of view.

Some researchers [1][2][3][4] experimentally investigated the critical height of combustible layer where detonation propagates successfully. They separated the combustible mixture and oxidizer or inert gas discontinuously with a plastic film. The critical height of hydrogen-air mixture layer is about three times as large as cell width. Reynaud et al. [5] simulates the detonation discontinuously stratified combustible and inert gas layers using one-step irreversible Arrhenius reaction model. They conclude that the critical layer height tends to be higher in accordance with the increment of activation energy. Houim et al.[6] numerically investigate the effect of the acoustic impedance ratio between combustible and inert gas layer by changing the temperature of the inert gas. The structure of the oblique shock and detonation front varies according to the acoustic impedance ratio.

Particularly considering a real situation, the interface of combustible mixture and oxidizer does not have a discontinuous concentration gradient. This difference may cause not only the mechanism of detonation propagation, but also the critical height of combustible layer. In this paper, the behavior of the detonation in stratified combustible mixture and oxidizer with concentration gradients is investigated.

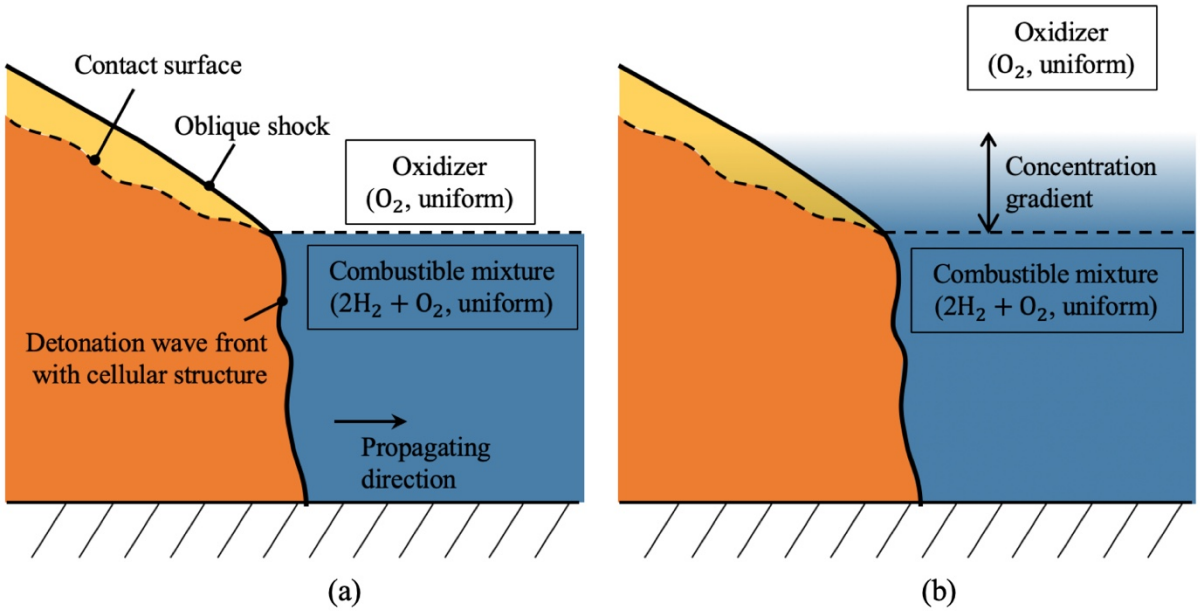

Figure 1. Schematic images of detonation in stratified combustible mixtureand oxidizer
(a) w/ concentration gradient (b) w/o concentration gradient

2.0 CALCULATION CONDITION

Fig. 1 shows schematic images of the calculation targets. Fig. 1 (a) is the case without concentration gradient, and Fig. 1 (b) is with concentration gradient. The composition of uniform combustible layer is $2H_2 + O_2$, and it of oxidizer is O_2. The concentration gradient between combustible mixture and oxidizer is defined by sigmoid function. Specifically, H_2 mole fraction is changed from about 0.66 (stoichiometry) to 0 by sigmoid function. In this study, the gain of sigmoid function is set as 0.04. Concentration gradient exists along 250 grid points (19.7 $l_{1/2}$). In w/o concentration gradient case, the gain is strengthened to 1. Therefore, the concentration gradient is almost discontinuous. The temperature of combustible mixture and oxidizer is 298 K, and pressure is 0.101325 MPa. The grid resolution is 3.5 μm. About 13 grid points include in half reaction length $l_{1/2}$ = 44.6 μm. Fig. 2 (a) shows the initial and boundary condition. High energy explosive is used for initial condition. The temperature is 3000 K, and the pressure is 10 MPa. The height of combustible layer h is static as h = 118 $l_{1/2}$. For reducing calculational cost, truncation method is used (see Fig. 2 (b)). The computational grid is moved to right when the detonation approaches the right boundary. The front of detonation is independent from any information behind the sonic line. Considering this structure of detonation, this operation for reducing calculational cost is effective. CJ velocity D_{CJ} is 2836 m/s, and the effective activation energy E_a / RT_{vN} is about 5.76. T_{vN} which is temperature at von Neumann spike is 1763.6 K.

$$\frac{\partial \hat{\mathbf{Q}}}{\partial t} + \frac{\partial \hat{\mathbf{E}}}{\partial \xi} + \frac{\partial \hat{\mathbf{F}}}{\partial \eta} = \hat{\mathbf{S}} \tag{1}$$

$$\hat{\mathbf{Q}} = \frac{1}{J}\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho_i \end{bmatrix}, \hat{\mathbf{E}} = \frac{1}{J}\begin{bmatrix} \rho U \\ \rho u U + \xi_x p \\ \rho v U + \xi_y p \\ (e+p)U \\ \rho_i U \end{bmatrix}, \hat{\mathbf{F}} = \frac{1}{J}\begin{bmatrix} \rho V \\ \rho u V + \eta_x p \\ \rho v V + \eta_y p \\ (e+p)V \\ \rho_i V \end{bmatrix}, \hat{\mathbf{S}} = \frac{1}{J}\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \omega_i \end{bmatrix}$$

$$U = \xi_x u + \xi_y v + \xi_t, V = \eta_x u + \eta_y v + \eta_t$$

$$e = \sum_{i}^{n} \rho_i h_i - p + \frac{\rho}{2}(u^2 + v^2) \tag{2}$$

$$p = \sum_{i} \rho_i R_i T \tag{3}$$

$$R_i = \frac{R_u}{W_i} \tag{4}$$

$$\frac{c_{pi}}{R_i} = a_{1i} + a_{2i}T + a_{3i}T^2 + a_{4i}T^3 + a_{5i}T^4 \tag{5}$$

$$\frac{h_i}{R_i T} = a_{1i} + \frac{a_{2i}}{2}T + \frac{a_{3i}}{3}T^2 + \frac{a_{4i}}{4}T^3 + \frac{a_{5i}}{5}T^4 + \frac{a_{6i}}{T} \tag{6}$$

$$\frac{s_i}{R_i} = a_{1i}\,ln\,T + a_{2i}T + \frac{a_{3i}}{2}T^2 + \frac{a_{4i}}{3}T^3 + \frac{a_{5i}}{4}T^4 + a_{7i} \tag{7}$$

The governing equations are two-dimensional compressible Euler equation with the conservation equations of 9 species (H_2, O_2, O, H, OH, H_2O, HO_2, H_2O_2, N_2) as it follows Eq. (1). Time integration for convective and source terms is separated based on fractional time step method. The ideal gas law is utilized to close the equations (Eq. (3)), and thermodynamic parameter is calculated by NASA polynomials [7] (Eq. (5) ~ (7)). The convective and source terms are separated by 1st order fractional time splitting. To discretize and integrate the convective term, AUSM-DV scheme [8] with fifth-order WENO [9] based on finite volume method and third-order TVD Runge-Kutta method are applied. The source term is integrated by Multi-Time Scale method [10] to avoid stiffness problem. Chemical reaction model includes 9 species and 20 elementary reactions [11].

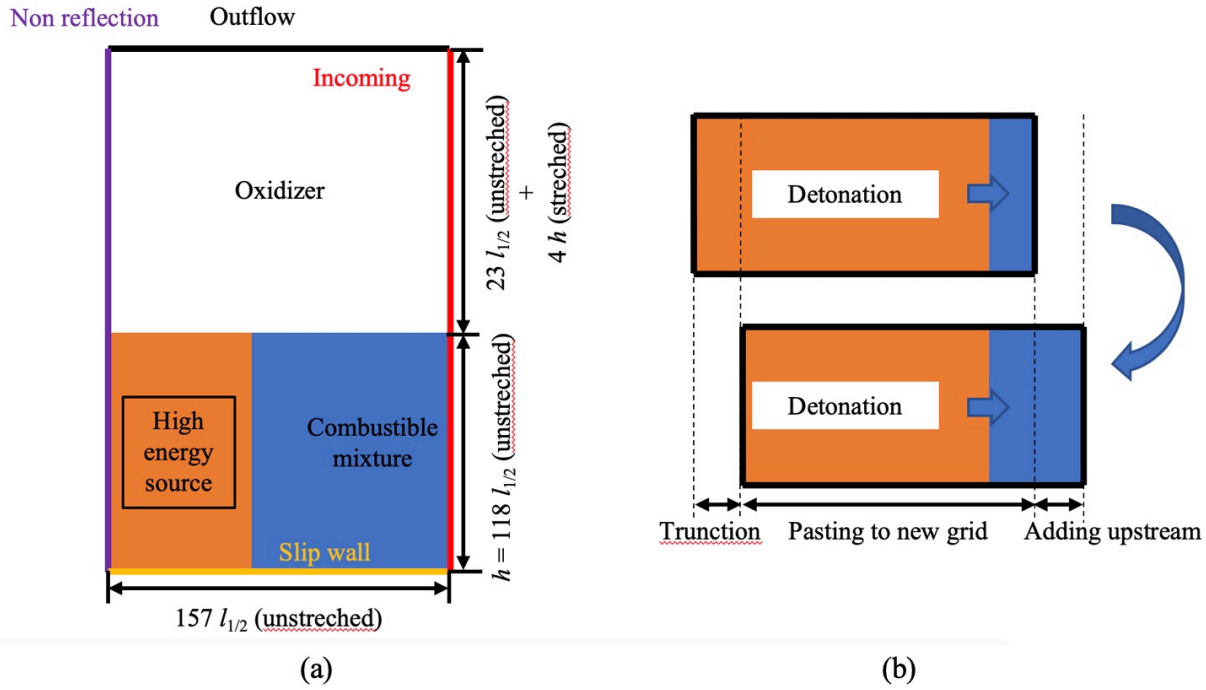

Figure 2. Schematic images of calculation condition
(a) initial and boundary condition (b) truncation method

3.0 RESULTS AND DISCUSSIONS

3.1 THE PROPERTIES OF DETONATION

Fig. 3 shows numerical maximum pressure histories of two cases without and with gradient. In without gradient case, cellular structure is irregular because the transverse waves do not reflect perfectly at the interface between combustible mixture and oxidizer (see Fig. 3 (a)). In addition to this, the trace of reflected shock is confirmed along the interface. The reflected shock is generated by difference of density behind the detonation front and the oblique shock. Mechanism that maintain the number of transverse waves moving downward is explained in a later part. In with gradient case, the reflected shock is not seen clearly within a region of non-uniform concentration (see Fig. 3 (b)). The number of triple points moving downward is generated less frequently than without gradient case. At last, detonation fails around $x/l_{1/2} = 1600$ with gradient case, whereas detonation propagates over $x/l_{1/2} = 3000$ in without gradient case.

Fig. 4 presents the history of the velocity at the bottom line. The velocity is calculated by differentiating the position of incident shock utilizing Savitzky-Golay filter [12]. The velocity fluctuation represents the fluctuations in cellular periods and the cellular irregularity. In contrast to without gradient case,

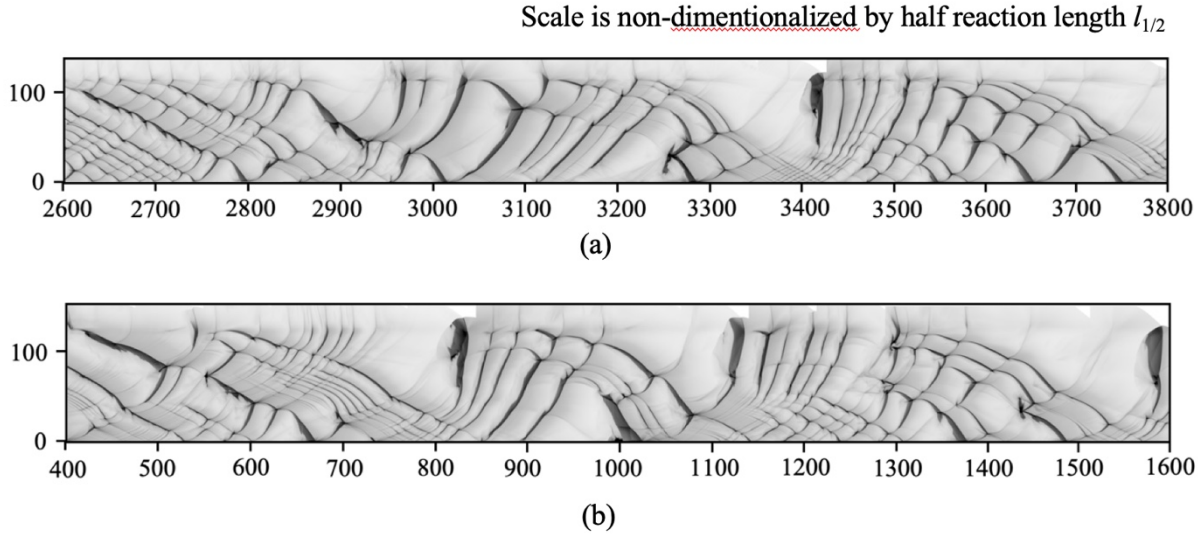

Figure 3. Numerical cell soot image (a) w/o gradient (b) w/ gradient

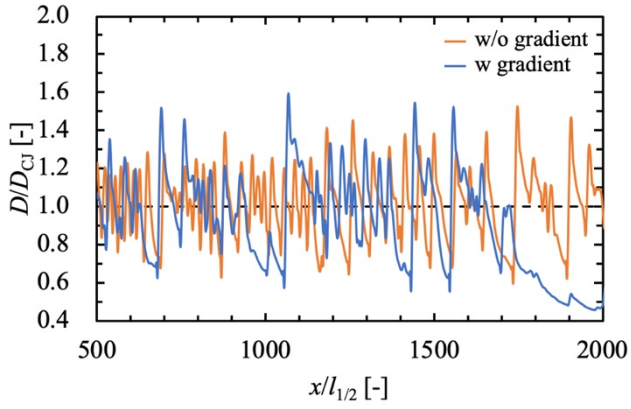

Figure 4. Propagating velocity along the bottom boundary

interval and amplitude of velocity fluctuation is not stable in with gradient case. This is because that the triple points moving downward is not generated periodically, and the local explosions along the bottom boundary occurs unstably. The section averaged velocity for $500 < x/l_{1/2} < 1600$ is 0.984 D_{CJ} in without gradient case, and 0.950 D_{CJ}. This difference is caused by temporary collapse of detonation structure and occurrence of transverse detonation.

Fig. 5 presents instant and averaged shape of the detonation fronts. The data of with gradient case is taken for $2600 < x/l_{1/2} < 3300$, and that of without gradient case is taken for $400 < x/l_{1/2} < 1100$. The averaged position is calculated by arithmetic mean of the position data along the same height y. The instant position of detonation front is concentrated upon the averaged position. In without gradient case, it seems that the instant position is concentrated more at the averaged position. Fig. 6 shows the averaged properties. The curvature of detonation front is obtained by approximating the averaged position with 3rd degree approximating polynomial. The approximating polynomials correspond well to the original averaged positions and their R-squared values correspond to 1 with an accuracy of 10^{-3}. The averaged positions and curvatures of detonation fronts are almost same between two cases (see Fig. 6 (a)). Fig. 6 (b) shows the curvatures of detonation are about zero around the bottom wall. Therefore, the velocity deficit is mainly not caused by the curvature of detonation front from the point of view of the averaged data. Fig.6 (c) represents the standard deviation of shock position which is taken from the data in Fig 5. The value of the standard deviation is almost the same between two cases around the bottom part. However, the value of without gradient case becomes lower than with gradient case as the height of the shock position increase. As previously stated, in with gradient case, the reflection of transverse waves is hard to occur at the interface of two kind of gas. Therefore, the fluctuation of shock position in with gradient case tends to increase. The averaged properties of detonation which is quenching does not change drastically by the existence of concentration gradient. However, the propagation distance of

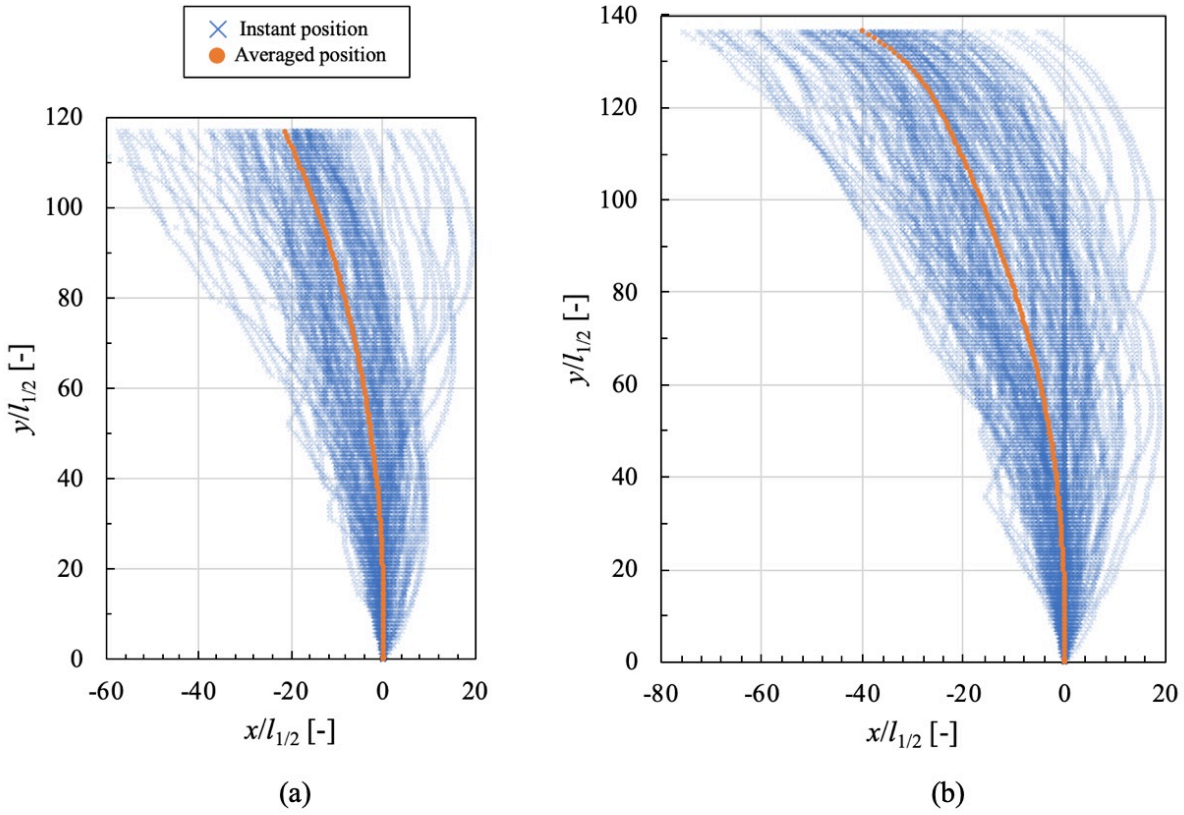

Figure 5. Instant and averaged position of the detonation fronts
(a) w/o gradient (b) w/ gradient

detonation is quite different. In the next section, the reason is investigated from the point of view of detonation behavior in micro scale.

3.2 MECHANISM OF DETONATION PROPAGATION IN MICRO SCALE

Fig. 7 presents a mechanism of occurrence of transverse waves moving downward in without gradient case. At first, transverse wave (written as TW in the figure) moves toward the interface between combustible and oxidizer layers (Fig. 7 (a)). The reflection of transverse wave is confirmed at the interface because the acoustic impedance changes discontinuously there (Fig. 7 (b), (c)). This phenomenon is one of the confined effects as the same way as the detonation propagates in a channel. On the other hand, the acoustic impedance ratio is not as high as between combustible gas and solid wall. Therefore, the detonation is separated as the transmitted shock in the layer of oxidizer and the reflected shock in the combustible gas. The reflected shock is not detonation because it does not have enough strength here. A next transverse wave moving upward approaches the reflected shock. Under this circumstance, an unburned gas pocket is formed between the reflected shock and transverse wave (Fig. 7 (d)). Finally, the unburned gas pocket is ignited by the transverse wave, and a new transverse wave moving downward arises (Fig. 7 (e)). These process cycles periodically. In other words, the number of transverse waves moving downward does not change drastically because this mechanism often occurs. The trace of this mechanism is also confirmed from Fig. 3 (a).

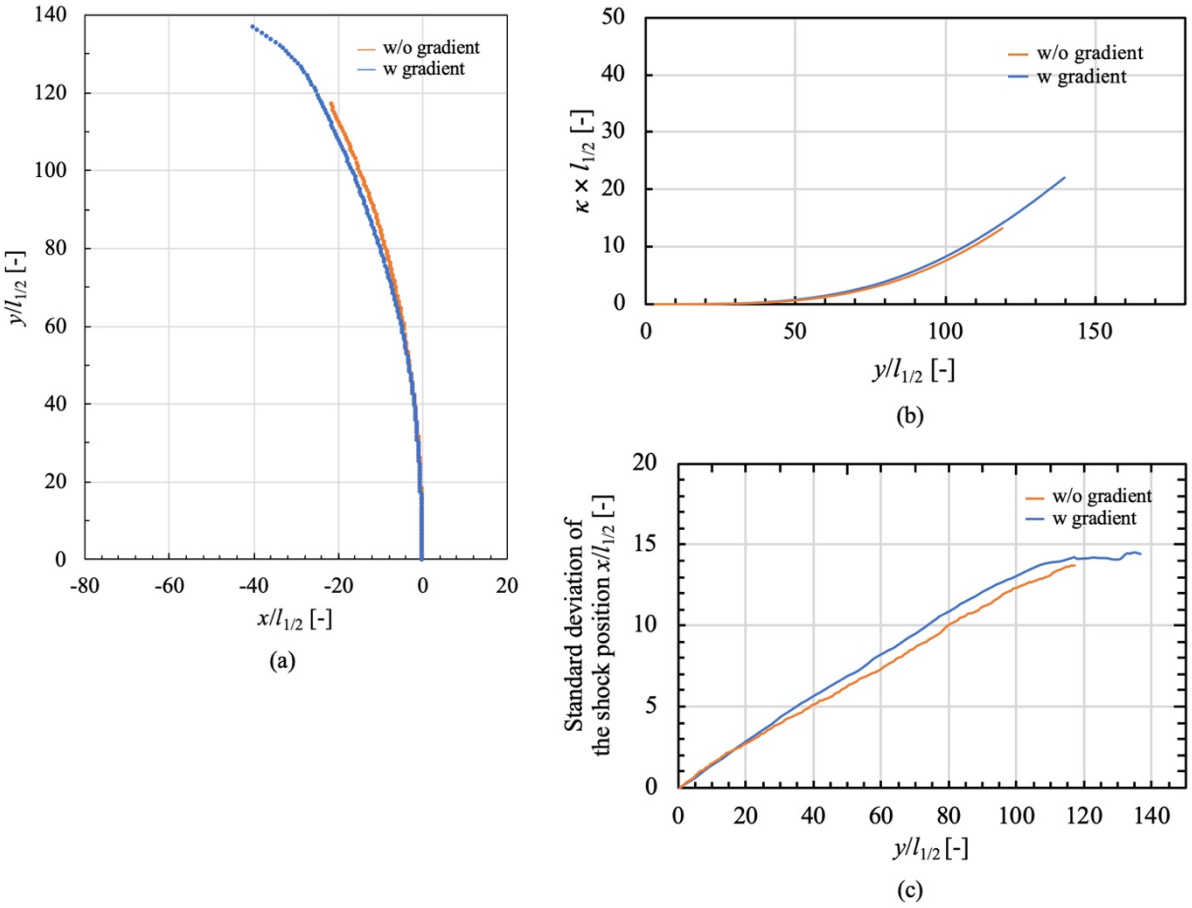

Figure 6. Comparison of averaged property (a) position (b) curvature (c) standard deviation of shock position

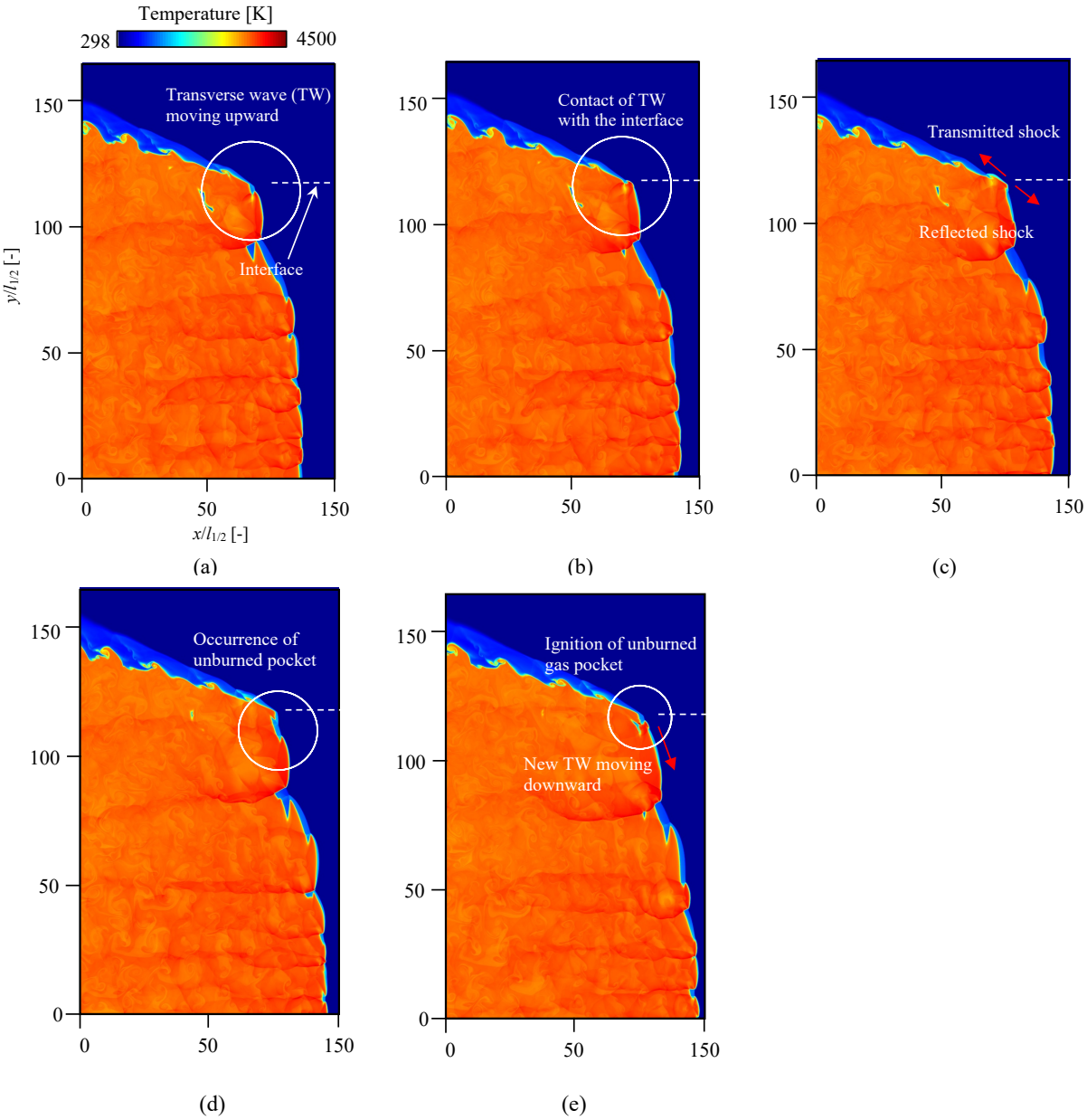

Figure 7. Mechanism of occurrence of transverse wave moving downward in without gradient case ((a) ~ (e) means passage of time)

Fig. 8 presents a behavior of transverse wave moving upward near the interface. Dotted line means the interface between uniform combustible gas (written as interface 1) and dot-dash line means the interface between the area with concentration gradient and the layer of oxidizer (written as interface 2). Firstly, a transverse wave moves into the interface 1 (Fig. 8 (a)). However, a reflected shock is not confirmed because there is almost no difference of the acoustic impedance ratio. The transverse wave is not reflected in the area with concentration gradient and interface 2 because of the same reason. Therefore, the transverse waves flow into the layer of oxidizer, and the enough transverse waves moving downward which makes detonation propagation stable does not occurs. This state is also confirmed in Fig. 2 (b), for example $x/l_{1/2} \approx 700$.

Fig. 9 shows a mechanism of the occurrence of transverse wave moving downward. Firstly, a huge transverse detonation propagates towards the buffer layer (Fig. 9 (a)). After that, a small disturbance occurs behind the transverse detonation before it reaches interface 1 (Fig. 9 (b)). Therefore, this

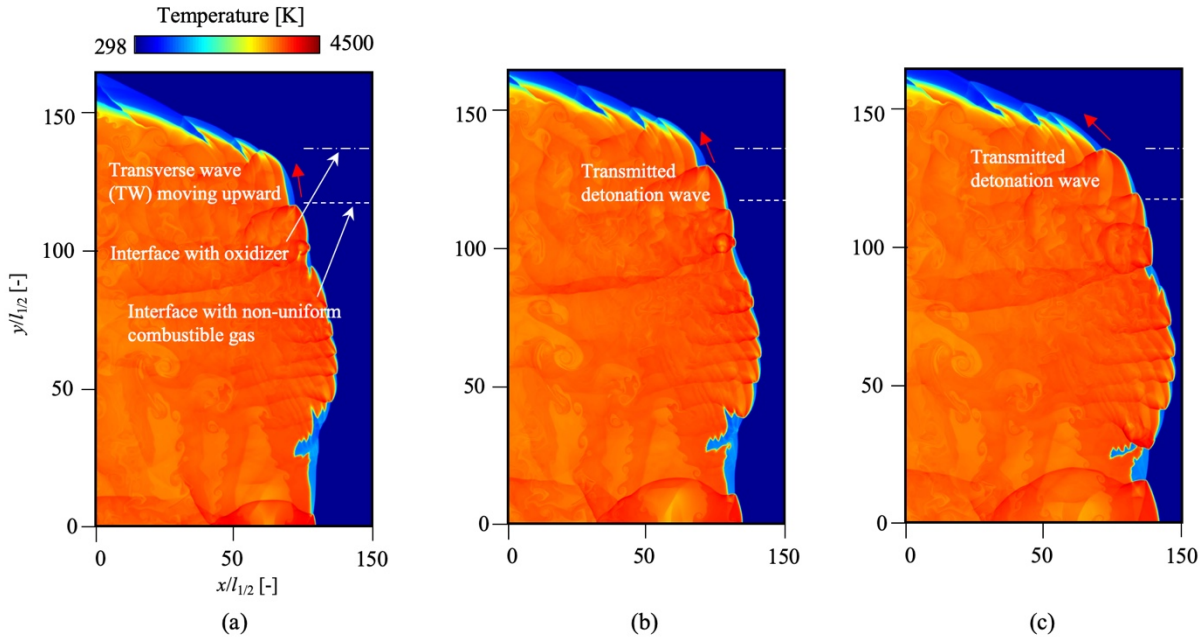

Figure 8. Behavior of transverse wave near the interface in with gradient case
((a) ~ (c) means passage of time)

disturbance is not caused by reflected shock. The disturbance and the next transverse wave collide with each other and make small local explosion. The local explosion makes a new transverse wave. Many of transverse waves moving downward occur after the transverse detonation in the maximum pressure history (Fig. 2 (b)). These mechanism in without gradient case does not contribute to sustain the stability of propagation because the transverse detonation occurs when the detonation

4.0 CONCLUSION

The detonation in stratified combustible mixture and oxidizer with concentration gradients is numerically investigated. In without gradient case, detonation propagates over $x/l_{1/2} = 3000$. On the other hand, detonation propagate about $x/l_{1/2} = 1600$ in with gradient case. Firstly, the properties of detonation in both cases when it is unstable are taken. The shapes of detonation fronts are almost same, and the averaged curvature along the bottom boundary is about zero. Therefore, the velocity deficit is not caused by the loss of curvature. The occurrences of transverse waves are focused to clarify the difference of stability. In without gradient case, transverse waves are reflected at the interface between two kind of gas because the acoustic impedance ratio changes drastically at the interface. The reflected shock wave and the other transverse wave collide and cause local explosion. This explosion generates a new transverse wave moving downward. In with gradient case, the reflection of transverse waves is rarely confirmed because the acoustic impedance does not change significantly at the interfaces. On the other hand, a new transverse wave moving downward is confirmed when the transverse detonation moving upward occurs. In other words, this generation does not occur when the detonation propagates stably. Therefore, the detonation with concentration gradient needs higher combustible layer height in comparison with the detonation without concentration gradient.

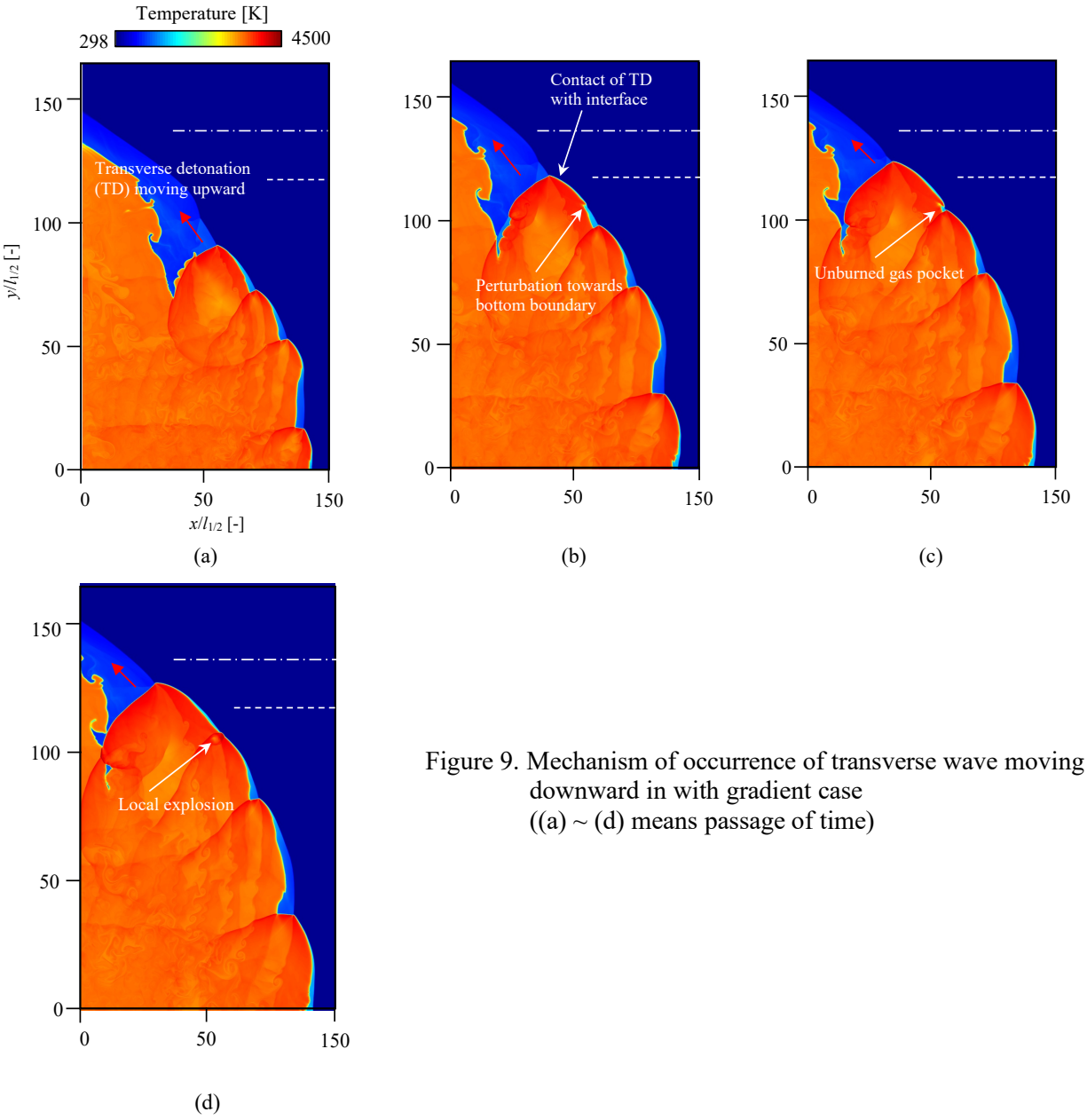

Figure 9. Mechanism of occurrence of transverse wave moving downward in with gradient case
((a) ~ (d) means passage of time)

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