

# The Effect of Radius of Curvature on the Detonation Propagating to the Unconfined Space

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## 1 Introduction

When a detonation propagates from a tube into an unconfined space filled with a detonable gaseous mixture, a diffraction of detonation occurs due to an abrupt change of cross-sectional area. The shape of the detonation wave changes from a plane to a curve and an expansion waves generated from the vertex of the exit attenuate a leading shock wave. As a result, reaction front is decoupled from leading shock wave[1-2]. If the tube diameter is smaller than the critical one, reaction front is completely decoupled from leading shock wave and the detonation wave fails to propagate into an unconfined space. On the other hand, if the tube diameter is larger than the critical one, re-initiation occur and the detonation wave succeeds to propagate into an unconfined space.

Some experimental and numerical researches have been conducted to reveal the characteristics of detonation diffraction. Khasainov et al. [3] revealed the effect of the divergence angle of the flow channel on the re-initiation process with a soot foil by changing the divergence angle from 5 to 90 degrees. When the divergence angle is smaller than 40 degrees, the re-initiation occur near the channel wall, however the divergence angle is larger than 40 degrees, the re-initiation is originated at tube axis. Arienti and Shepherd [4] conducted numerical simulation about the effect of the activation energy on detonation diffraction with single-step chemical reaction model in Arrhenius form and clarified the detonation diffraction is affected by the activation energy. Nagura et al. [5] conducted an experiment by varying the composition of mixture and divergence angle from 30 to 150 degrees. They revealed that the diffraction behavior is similar for two mixtures and it is roughly defined by cell width. Nakayama et al. [6] investigated the propagation behavior in a curved cross section, where the detonation wave is supported by the effect of outer wall. They showed that  $R_{in}/\lambda$  is an important parameter to determine the criterion for the propagation of the stable detonation wave. In their study, propagation of the detonation wave is supported by the effect of outer wall.

This study focuses on two-dimensional diffraction of detonation wave propagating in the confined channel, and the numerical investigation is carried out in two-dimensional space. The aim of this study is to clarify the effect of the radius of curvature on detonation diffraction with expanding diffraction surface without support by the outer wall. The effect is examined using the soot track images, distribution of flow variables, and the shock pressure histories, and the criterion for the propagation of the stable detonation wave is indicated based on the simulation results.

## 2 Numerical Setup

In this study, the compressible and reactive two-dimensional Euler equations are used as governing equations and the fluid is assumed to be an ideal gas with constant specific heat ratio. The two-step reaction model proposed by Korobeinikov et al. [7] is used for chemical reaction. This model represents induction and exothermic periods with induction progress variable  $\alpha$  and exothermic progress variable  $\beta$ . The reaction rate for each periods are shown in the following equations.

$$\omega_\alpha = -\rho k_1 \exp\left(-\frac{E_1}{RT}\right)$$

$$\omega_\beta = \begin{cases} 0, & (\alpha \geq 0) \\ -k_2 \left[ \beta^2 \exp\left(-\frac{E_2}{RT}\right) - (1-\beta)^2 \exp\left(-\frac{E_2+Q}{RT}\right) \right], & (\alpha < 0) \end{cases}$$

where  $k_1$  and  $k_2$  are reaction rate constants,  $E_1$  and  $E_2$  are activation energies, and  $Q$  is heat release.  $p$ ,  $\rho$ ,  $R$ , and  $T$  indicate pressure, density, gas constant, and temperature respectively. In this study, chemical reaction parameters are set to be the same as those of Inaba [8] and premixed gas is modeled as stoichiometric hydrogen/air. Initial pressure and temperature of premixed gas are set to be 1atm and 293K, respectively. In these condition, the cell width equals to  $\lambda = 1.6$  mm.

As discretization methods, Yee's non-MUSCL type second-order upwind total variation diminishing scheme is used for the spatial integration, and a point-implicit method is used for time integration for source term. Figure 1 shows the computational target and domain in this study. The computational target is composed of the straight channel section, expanding channel section and unconfined space.  $R_c$  and  $L$  denote the radius of curvature of the expanding channel section and width of straight channel section, respectively. The ratio of  $R_c$  and cell width  $R_c/\lambda$  is varied from 0.06 to 20 to discuss the effect of radius of curvature on the behavior of detonation diffraction. The straight channel width is fixed at ten times the cell width in this study. The computational grids and boundary conditions in the case of curvature of radius is equal to  $R_c = 10\lambda$  are shown in Figure2. In this study, two types of grids are used; one is corresponding to an unconfined space and the other is corresponding to the diffraction wall. The physical values are exchanged between each grids. The grid resolution in the whole region maintains at least ten points in the induction zone length. Two dimensional well developed detonation in two dimensional straight channel is put at straight channel section as initial condition.

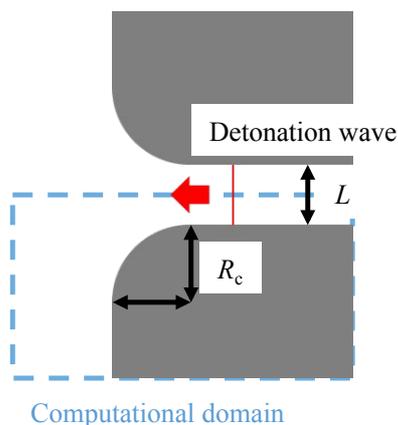


Figure 1. The schematic image of computational target and domain

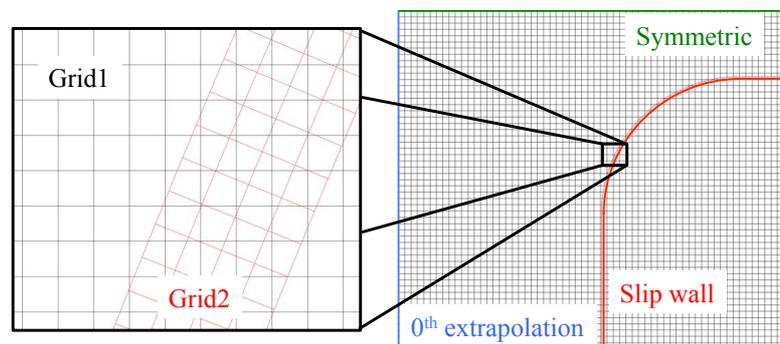


Figure 2. Example of computational grids and boundary condition in the case of the radius of curvature is equal to  $10\lambda$ .

### 3 Results and discussion

In the simulation results, two types of propagation behavior are observed depending on the radius of curvature: one is sub-critical regime and the other is super-critical regime. In order to see the characteristics of propagation behavior, soot track images generated from the maximum pressure histories are shown in Figure 3. See the soot track images in Figure 3, the cellular patterns are triangularly recorded near the straight channel exit regardless the radius of curvature. It means that the expansion effect originated from diffraction of channel wall attenuates the transverse waves toward the channel wall. Figure 3(a), (b), (c) and (d) seems to be categorized into sub-critical regime because of the detonation failure as observed in soot track images, although, in the case of  $R_c = 5\lambda$ , the local explosion is observed in Fig. 3 (c). Figure 4 shows instantaneous pressure and density distribution in each radius of curvature at the latest time. In Figure 4 (a), (b), (c) and (d), the triple points are attenuated and the leading shock front and reaction front are decoupled almost the entire wave front. As radius of curvature increases, the range of attenuation becomes small. Therefore, the transverse wave near the channel center is activated, and the cellular pattern expands toward the open area after the channel exit. Eventually transverse detonation waves generated near the tip of triangular area hit the curved wall, the reflected transverse waves propagate toward the center of channel, as observed in Fig. 3 (e) and (f). See Fig 3. (f), strong re-initiation is originated on the center of channel, which looks like a behavior of direct initiation of detonation. The time development images of pressure and density distributions in the case of  $R_c = 20\lambda$  are shown in Figure 5. The following explanation about re-initiation processes are corresponding to Figure 5 (a), (b) and (c).

- (a) The leading shock wave and transverse waves are attenuated by the expansion wave and decoupled from the reaction front on detonation front.
- (b) Triple points reflected from the channel wall are collision and local explosion occurs on the central channel axis.
- (c) Transverse detonation is generated due to the local explosion and propagates in shocked but unburned mixture. New triple points are formed on the detonation front after the propagation of transverse detonation wave.

After the re-initiation, new triple points are generated due to propagation of transverse detonation wave and they propagate on the detonation front as shown in Figure 4 (e) and (f). So, the wave front can be said that it is a fully developed to the detonation wave.

Figure 6 shows the pressure histories in sub-critical regime on (a) the center of channel and (b) the wall. The location of  $x = 0$  is corresponding to the exit of straight channel. Since the leading shock experiences the triangular area after the confined channel, the behavior of the pressure histories on the center of channel in Fig. 5 (a) is identical at  $-13 < x < 0$  in Figure 6 (a). Although the behavior depends on the radius of curvature at  $x < -13$ , the pressure oscillations finally disappear in the pressure histories. Regarding the pressure histories on the wall in Figure 6 (b), the effects of wall curvature appear immediately after the confined tube, and the behavior strongly depends on its curvature. The pressure oscillation finally calms down, although the larger radius of curvature takes longer time. Figure 7 shows the pressure histories in super-critical regime on (a) the center of channel and (b) the wall. As well as Figure 6 (a), the pressure histories are identical at  $-18 < x < 0$ , where the leading shock passes through the triangular area in Figure 7 (a). After that, the oscillation behavior is different each other due to the scale of curvature showed up into the behavior of oscillation, and the unstable oscillation never stops. The oscillation behavior on the wall in Figure 6 (b) shows the same trend as well as Figure 6 (a).

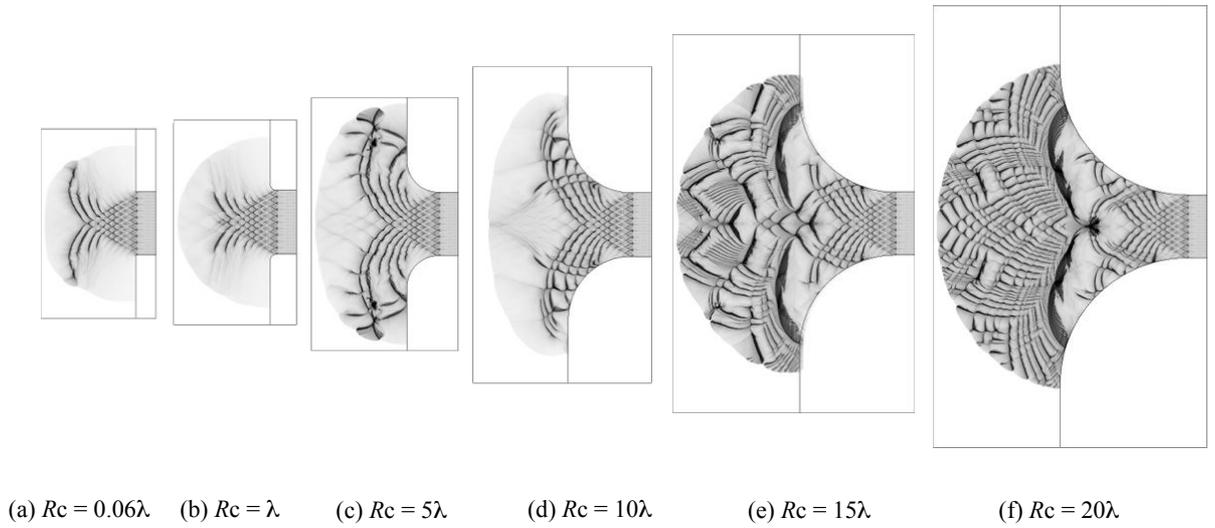


Figure 3. Soot track images generated by maximum pressure histories.

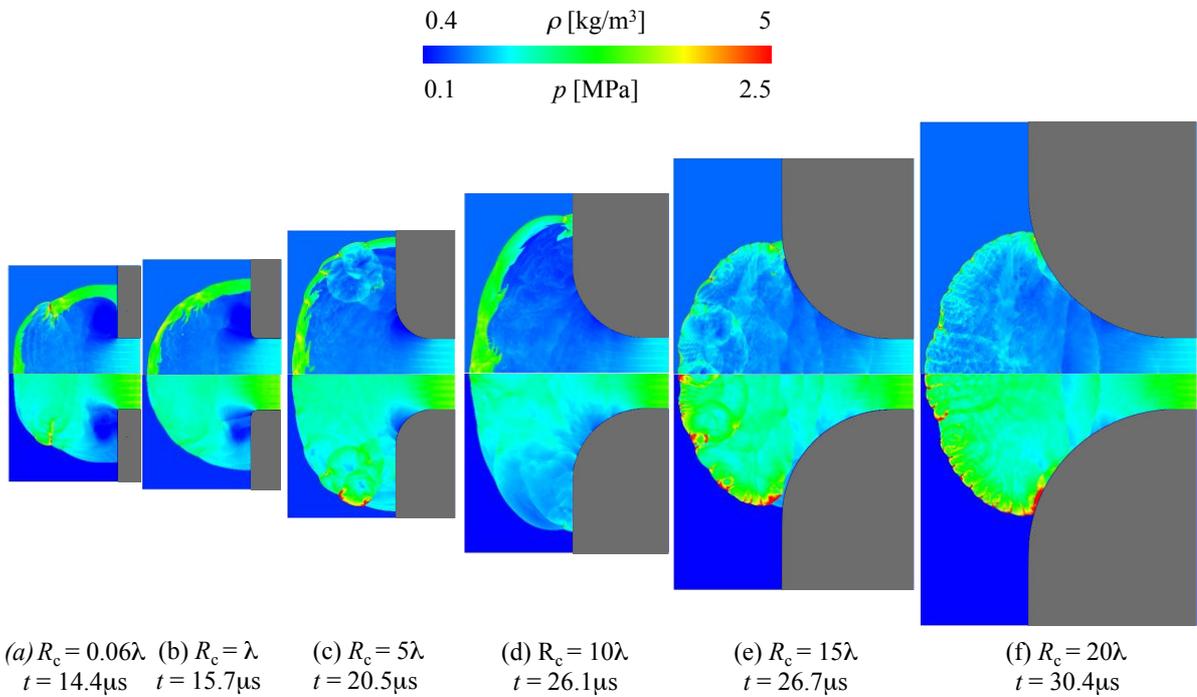


Figure 4. The instantaneous pressure and density distributions in each radius of curvature at the latest time.

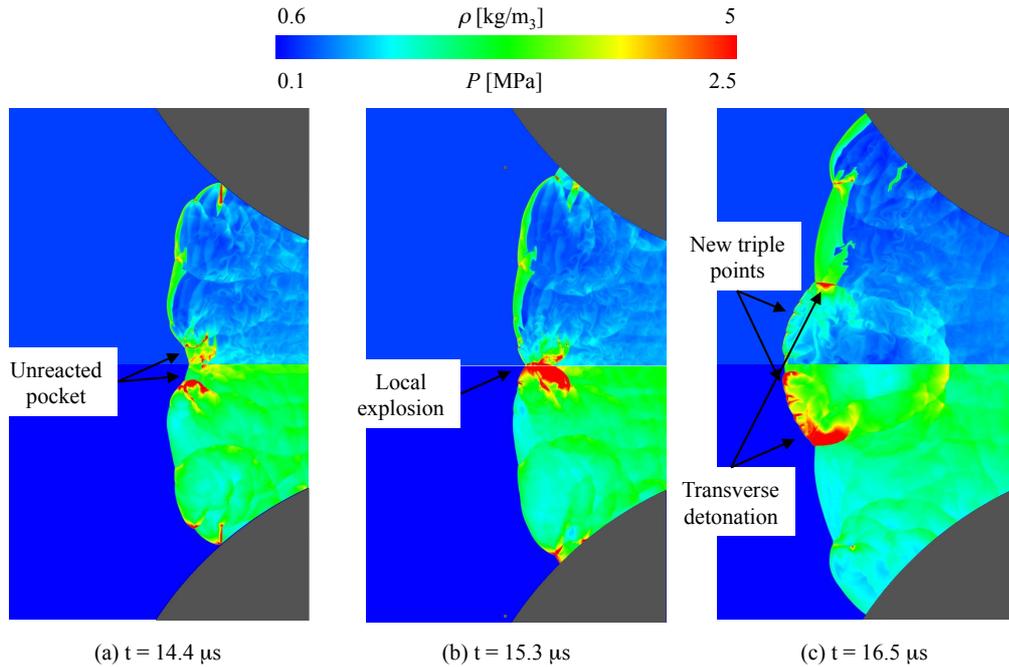


Figure 5. Temperature and density distribution in the case of  $R_c = 20\lambda$  when the local explosion occurs.

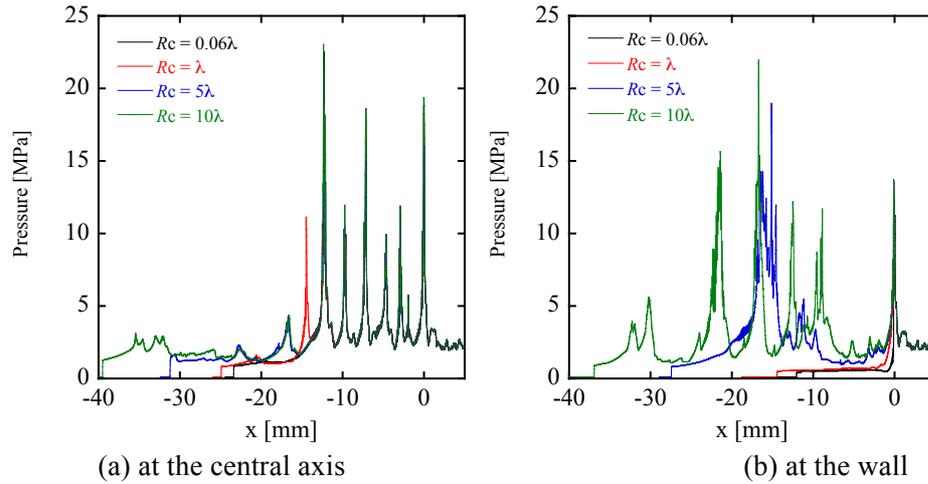


Figure 6. Shock pressure histories in the case of sub-critical regime.

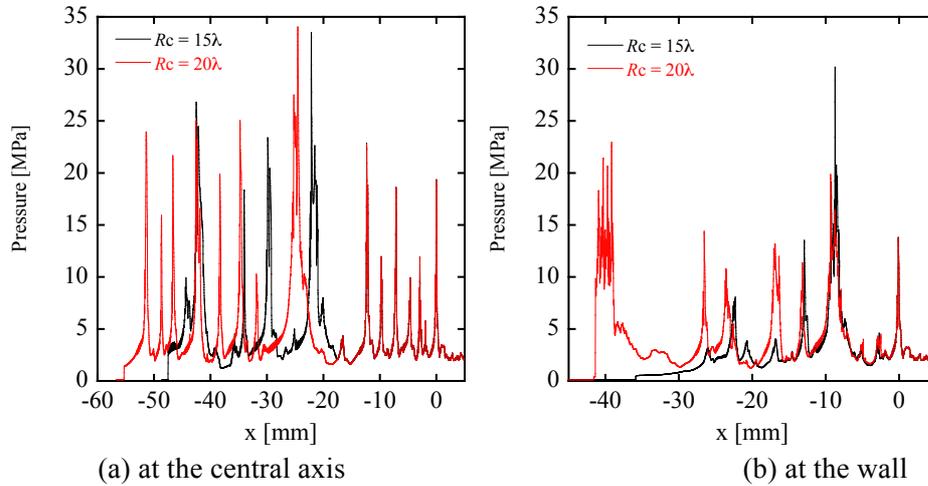


Figure 7. Shock pressure histories in the case of super-critical regime

## 4 Conclusions

Two-dimensional detonation diffraction along the curved diffraction surface from straight channel to unconfined space was numerically investigated by using two-dimensional Euler equations and a two-step chemical reaction model proposed by Korobeinikov et al. The straight channel width was set to be five times cell width and the radius of curvature was varied from  $0.06\lambda$  to  $20\lambda$  to confirm the effect of curvature on detonation diffraction. The propagation behavior changed from sub-critical regime to super-critical regime as increase of the radius of curvature and the critical value was  $R_c = 15\lambda$ . In sub-critical regime, the leading shock wave and the reaction front were decoupled and failed to propagate into the unconfined space because the expansion effect was too strong to maintain the cellular structure. In super-critical regime, the local explosion occurred due to collision of reflected triple points. The transverse detonation was generated by local explosion and propagated toward the wall. New triple points were formed after propagation of the transverse detonation and succeeded to propagate to the unconfined space. It implies the existence of the critical radius of curvature for the stable propagation of detonation and that the curved inner wall supports the detonation wave in the unconfined space.

## References

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