Numerical Study on Re-Initiation of Detonation Propagating through Double Slits in a Planar Channel

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1 Introduction

For the safety of flammable gas transports and handling, suppressing the detonation wave is an important demand for the industry related to flammable gas handling. In particular, one way of detonation quenching is diffraction. Sudden expansions during the detonation propagation decrease the temperature and contribute to reducing reaction rates and separating the shock wave and reaction front. According to Mitrovanov and Soloukhin [1], the critical diameter for the detonation extinction is 13λ for a circular tube and 10λ for a planar channel, where λ is the equilibrium transverse wave spacing. Despite the decoupling of shock and reaction fronts due to diffraction, detonation waves still can be re-initiated once a high-energy source exists downstream such as Mach reflection [2-4]. Ohyagi et al. [5,6] show experimentally that diffracted two shock waves from double slits also re-initiates the detonation wave. Moreover, they suggested that re-initiation distance and re-initiation mechanisms can be correlated with non-dimensional distance, where w is the width of slits. The w/λ ratio greater than unity was a favor for shock-shock re-initiation, which means at least one cell emerges at the slit. If w/λ is smaller than unity, diffracted shock-shock interaction fails to produce the detonation wave, and shock-wall or reflected shock-shock interaction can be the next candidates of detonation re-initiation. However, detailed processes of shock-shock re-initiation are still questions and need to be investigated to understand the detonation re-initiation fully.

In the present study, numerical simulations on a stoichiometric hydrogen-oxygen detonation reinitiation process of planar channels with double slits were performed to examine the diffracted shockshock re-initiation process in detail. Shock-shock re-initiations were demonstrated by the CFD solution based on previously reported experimental work [5,6].

2 Numerical Method

The reacting compressible Navier–Stokes equations were considered. In the finite volume approach, equations of mass, momentum, energy, and species conservations were solved based on the OpenFOAM platform [7], with the ideal gas equation of state. For the flux evaluation, the HLLC scheme was applied with van Leer limiter and time integration was performed by the TVD 3rd-order Runge-Kutta method. For the mixture of hydrogen and oxygen, a detailed hydrogen oxidation mechanism [8], namely San Diego mechanism, was considered, including 11 species and 23 reactions. The two-dimensional computation domain is given in fig.1. Double slits are located in the detonation tube. The detonation tube has 50 mm width for the detonation propagation region and slit width is 8 mm with a distance between slits of 10 mm. These configuration and geometry correspond to the one of previously reported experiment setup [5,6]. The grid resolution can be important for the present study, to capture the physics of local detonation extinguish and re-initiation processes. In particular, a downstream cell size of 20 μm was considered for the stoichiometric hydrogen and oxygen mixture of its pressure as 25 kPa. To reduce

the computation cost, upstream cell size was chosen as $100 \ \mu m$ and initial profiles of detonation were derived from one-dimensional Chapman-Jouguet detonation (u_{CJ} =2794 m/s) results which were calculated by the same numerical method maintaining identical numerical viscosity. Various initial pressures (10-40 kPa) of the tube have been studied, whereas gas temperature was fixed as 300 K. Isothermal (300 K) and no-slip boundary conditions were applied at the walls.



Figure 1: Schematic diagram of the two-dimensional planar channel with double slits

3 Results and discussion

Once shock waves are diffracted, rarefaction waves can decouple the shock wave and reaction front. Figure 2 shows numerical schlieren and mass fraction contour of OH species of the diffracted detonation wave. Typical flow patterns of shock wave diffraction such as expansion fan, shear layer, secondary shock, and vortex can be observed. Separation of reaction front and shock wave dominates in strongly diffracted regions. Once again, the mass fraction of OH species shows that the reaction front is decoupled from the shock wave.



Figure 2: Numerical schlieren and mass fraction contour of OH species of the diffracted detonation wave, $p_0 = 25 \text{ kPa}$

Figure 3 shows sequential numerical schlieren of the shock-shock re-initiation process. Initially, diffracted shock waves start to interact at the center of slits and generate local explosion shock waves $(t=1 \ \mu s)$. Then, explosion shock waves followed by reaction front propagate to the downstream $(t=2 \ \mu s)$ and produce an energy source to initiate the detonation wave. Finally, the re-initiated detonation wave propagates downstream $(t=2-11 \ \mu s)$. Figure 4 shows downstream pressure along the y=0 line. At t=0.57 μs , a sharp pressure peak exists, due to the interaction between two diffracted shock waves.

Daeyoung Jun

Numerical Study on Detonation Re-Initiation



Figure 3: Sequential numerical schlieren of the shock-shock re-initiation process, $p_0 = 25$ kPa

Two explosion shock waves propagating to the opposite directions are observed (t= $0.57-2.01 \ \mu s$) and shock wave propagating to the downstream initiates the detonation wave. After that, pressure level is approaching to ZND pressure.

Downstream pressure along the y=0 line



Figure 4: Downstream pressure profiles along the y=0 line, $p_0 = 25$ kPa

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Daeyoung Jun

Numerical Study on Detonation Re-Initiation

Figure 5 shows the downstream mass fraction of OH species and pressure profiles along the y=0 line. The solid line is pressure and the dotted line is the mass fraction of OH species. Initially (t=0.57 μ s), the reaction front is decoupled from the incident shock wave and the explosion shock wave is far behind the reaction front. However, explosion shock wave (3620 m/s) toward downstream propagates faster than the reaction front (2070 m/s) and incident shock wave (2320 m/s), so they finally merge (t=1.56 μ s) initiating the detonation wave. These suggest that explosion shock wave is very important to understand the shock-shock reinitiation process of the double slits.

4 Conclusion

In the present study, numerical simulations on the detonation reinitiation of the planar channel with double slits were performed in order to examine the diffracted shock-shock re-initiation process in detail. Diffracted shock waves produce explosion shocks and these energetic waves propagate faster than reaction front and incident shock wave and finally initiate the detonation wave. It is found that explosion shock waves play an important role in shock-shock re-initiation of the detonation wave, which is in agreement with the previously reported experiment [5,6].



Figure 5: Downstream mass fraction of OH species and pressure profiles along the y=0 line, $p_0 = 25$ kPa

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