Roughness Influence on Flame and Detonation Propagation

Edyta Dziemiska, Yuto Hara, Mitsuharu Morishita Faculty of Science and Technology, Sophia University Chiyoda, Tokyo, Japan

1 Introduction

In this study, experiments as well as numerical simulations of flame, detonation, and deflagration-todetonation transition (DDT) were performed to find how surface roughness in micro-scale effects combustion processes and what the smallest roughness that can be a reason for detonation is, which can mean either shorter detonation initiation distance (DID) or induction time. Modeling was done with the twodimensional channel with boundary conditions of different wall roughness (Ra) from 0 (smooth) to 0.8 μ m, 1.6 μ m, 3.2 μ m, and 1mm. The numerical results show a process of DDT under all conditions and furthermore, some characteristics of detonation.

2 Background

Currently, interest in hydrogen research as an alternative energy source are progressing. While the realization of technology using hydrogen is developing, hydrogen is hiding the potential of an unexpected explosions and potential danger. We want to introduce research that have not been yet conducted on how a small change of surface roughness can speed up and change characteristics of detonation propagation.

It is well known that surface roughness generates turbulence and leads to detonation. DDT can occur faster and spreads detonation limits with bigger roughness. However, until now there was not much study done on the lower limit for DDT dependence on roughness unlike obstacles. The turbulence that is generated by rough tube wall favors flame acceleration and speeds up the detonation process, namely, occurrence of turbulence makes it easy to cause detonation. A lot of studies on deflagration-to-detonation transition in obstructed channels have been performed [1-9], but there is almost not studies on roughness in micro scale.

Ra, which is one of the ways to indicate roughness, is an arithmetic average of the absolute values of roughness profile ordinates and it is expressed in micrometer (μ m) (Figure 1). The present processing technology is able to manufacture surface roughness up to 0.8 μ m. Therefore, we chose this scale which is to be standard change in roughness value for this research.



Figure 1. Roughness measurements, where Ra - arithmetic average roughness, m – center line, l – measurement length.

3 Initial conditions

Numerical analysis was performed using OpenFOAM and the DDT phenomenon was calculated with ddtFOAM solver. The reason to use OpenFOAM is the ability to simulate DDT in 2D with wall function describing microstructure of wall.

Figure 2 shows the size of the model, boundary conditions, and Table 1 initial conditions. Calculation domain is set to be the two-dimensional channel of 3.8 mm and length of 3000 mm with roughness on top and bottom walls (Ra) of 0 μ m (smooth), 0.8 μ m, 1.6 μ m, 3.2 μ m, and 1mm. The chemical reaction model is built with nine species (H₂, O₂, N₂, H, O, OH, HO₂, H₂O₂, and H₂O) and 21 reactions.



Figure 2. Calculation domain

Table	1.	Initial	conditions
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	Ignition Region	Ambient Region	
Temperature [K]	2448	293	
Pressure [MPa]	0.1	0.1	
Mixtures	Stoichiometric H ₂ /Air		

4 Experimental setup

Square detonation tube (38x38 mm) consists of 6 parts 500 mm length each, where one part consists of 400 mm observation window. Flow visualization is done with Schlieren system and high speed camera (Figure 3). Premixed hydrogen air mixture was used in the experiment. So far results were only obtained for tube with roughness of $0.8 \mu m$.

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Figure 3. Phantom camera (640x192 and 160 000 fps) used for experiments.

5 Results

Deflagration to detonation transition occurred at about the same time and the same distance under conditions of $Ra = 0 \mu m$ (smooth), $Ra = 0.8 \mu m$ and $Ra = 1.6 \mu m$. It could be confirmed that about 5 % shorter induction time and up to 8 % shorter DID occurred with $Ra = 3.2 \mu m$. And with Ra = 1 mm about 12 % shorter induction time and up to 15 % shorter DID was seen. Thus, the smallest roughness which affects detonation phenomenon should be between $Ra = 1.6 \mu m$ and $Ra = 3.2 \mu m$. In other words, the micro scale roughness effects are significant in DDT phenomenon. Figure 5 summarizes numerical finding, however, more detailed calculations are required. We hope to confirm the same findings with further experiments. Figure 4 illustrates one frame of high speed camera movie taken during the experiment. Calculation model is exactly 10 times smaller than experimental tube and with the same mixture at least we could observe propagating detonation.



Figure 4. Propagating detonation.



Figure 5. Flame front velocity for different wall roughness.

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