Explosive Transition of Deflagration in PRF/air Mixtures

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1   Overview

Engine knock poses a significant challenge in the development of high-efficiency spark ignition (SI) engines, as it diminishes the engine performance and can cause severe damage on engines. Extensive research has been conducted to understand knock onset and improve engine efficiency.

Traditionally, the Livengood-Wu integral based on ignition delay time has been used to predict engine knock, but understanding the behavior of deflagration waves under high pressure and temperature conditions is also crucial to unravel the knock mechanism. In such conditions, the role of chemical reactions in the preheat zone of deflagration becomes more significant. For example, low-temperature oxidation, observed in fuels like n-heptane, strongly influences flame characteristics [1].

Recently, theoretical and numerical analysis was performed to investigate the relationship between 0D homogeneous ignition and 1D laminar premixed flames at various Lewis numbers [2]. This study revealed that when the Lewis number exceeds unity, the 1D laminar premixed flame structure can no longer be sustained beyond a certain inlet temperature due to autoignition predominating in the preheat zone. This vanishment of the 1D flame structure was termed as "explosive transition of deflagration" [2].

Another key factor used to understand engine knock is the octane number. It is empirically known that the octane number indicates fuel's anti-knock characteristics and is defined as the volumetric proportion of iso-octane in Primary Reference Fuel (PRF), a blended fuel of n-heptane and iso-octane.

The objective of this study is to investigate the effect of octane number on the "explosive transition of deflagration". As a first step, the limit temperature for "explosive transition of deflagration" was examined for various ratios of iso-octane in the PRF.

Numerical simulations of 1D laminar premixed flames were conducted using Cantera ver. 3.0.0b1 [3]. PRF/air mixtures were utilized, and a SIP reduced model [4, 5] was used as the detailed reaction mechanism. The initial pressure and equivalence ratio were fixed at 4.0 MPa and 1.0, respectively. The ratios of iso-octane in the PRF were varied from 0 to 100. The simulations varied the inlet temperature from 300 to 1500 K, and the inlet temperature at which the simulation failed was defined as the threshold temperature of "explosive transition of deflagration" (T_{ETD}). The precision of T_{ETD} was 1 K. The

computational domain should be as short as possible since the solutions of 1D laminar premixed flames under elevated temperature (and pressure) conditions are domain dependent [2, 6].

In all conditions of iso-octane ratio in the PRF, "explosive transition of deflagration" was observed, consistent with the theoretical analysis for Lewis number greater than 1. T_{ETD} ranged from 1151 K to 1254 K, and generally increased with increasing number of PRF.

This presentation will also provide the progress of an ongoing experimental work to elucidate the knock onset mechanism using a constant volume chamber.

Note that the behaviors of deflagration wave near "explosive transition of deflagration" for stretch-free planar flame and for stretched flame will be presented in this conference [7] and [8], respectively. The relationship between "explosive transition of deflagration" and practical engines will be presented in the Plenary Lecture by Professor Kaoru Maruta in this conference, too [9].

References

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