学 位 論 文 内 容 の 要 旨

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学 位 論 文 題 名

A Study on Low-temperature Ignition of DME-air Mixture at Atmospheric Pressure

(DME 混合気の常圧下における低温着火に関する研究)

Dimethyl ether (DME: $CH_3OCH_3$) has been considered as a promising alternative fuel due to its merits of favorable compression ignition property and little soot formation in combustion field. A deep understanding of low-temperature ignition of DME is important in two engineering aspects: the design of engine and the safety for preventing accidental explosions. The ignition of DME exhibits a two-stage mode, which shows complexity due to the existence of the negative temperature coefficient (NTC) effect. Further investigation to elucidate the characteristics of low-temperature ignition of DME is needed especially at atmospheric pressure. The objective of this study is to develop an experimental system that could capture low-temperature ignition process of DME. Special attention will be given to the transition from a cool flame to a hot flame. Furthermore, the existing ignition kinetics model of DME is expected to be validated using the developed system. Suggestions based on the validations are expected to be proposed to improve the DME ignition kinetics.

In Chapter 1, first, significance of research on low-temperature ignition as well as the two-stage ignition regime is introduced. Then, previous studies on DME ignition kinetics are briefly summarized. Finally, objective and scope of this dissertation are shown.

Chapter 2 shows the first attempt to capture low-temperature ignition of DME, which is conducted in a straight 1400 mm long Pyrex flow reactor. The observed periodic behaviors with ignition, flame propagation, and extinction are interpreted. Two distinct flames, weak flame and hot flame, are identified. The weak flame is found to transit to the hot flame with the decreasing of equivalence ratio. Time sequential analyses are conducted, indicating that the intermediates formaldehyde, methyl formate and formic acid, formed due to the mild oxidation, are completely consumed by the hot flame.

In Chapter 3, in order to achieve clear observation of flame motions, the flow reactor is then updated into a transparent one. Thanks to the updated reactor, the mechanism of the periodic weak flame behavior is clarified. It is indicated that the weak flame occurrence is accompanied by the formation of intermediate product species, such as formaldehyde and methyl formate. Therefore, the weak flame might be cool flame, or flame formed due to the significant suppression of the transition from a cool flame to a hot flame. Moreover, it is found that the ignition disappears at above 590 K, indicating the

negative temperature coefficient (NTC) zone is encountered. Gas analyses are conducted toward the periodic flame behaviors in the ignition regime, as well as the stable oxidation conditions in the NTC zone. The results are further discussed based on the detailed chemical kinetics. It is proposed that a new chain-propagation pathway might exist via the decomposition of the species HPMF (hydroperoxy-methyl formate, $HOOCH_2OCHO$) and be pronounced at above 540 K, which suppresses the transition from the cool flame to the hot flame.

In Chapter 4, to investigate the ignition kinetics, numerical computations are performed using a plug-flow model accounting for heat transfer between the gas mixture and the reactor. This model predicts well the ignition limit in experiments, however, fails to predict the transition from a cool flame to a hot flame. Reaction pathway analyses results suggest that the competition between the $\beta$-scission reaction and the molecular oxygen addition reaction of the methoxy-methyl radical ($CH_3OCH_2$) could strongly influence the transition. This influence is further investigated via a slight modification of the activation energy of the $\beta$-scission reaction of the $CH_3OCH_2$ radical. Depending on this modification, both the ignition limit and the ignition regimes against equivalence ratio are well predicted: a two-stage ignition regime corresponds to a hot flame in the experiments, and a transition suppressed ignition regime corresponds to a weak flame in the experiments, respectively. In addition, the kinetics model with this modification shows reasonable agreement with shock tube ignition delay results. It is shown that the modification strongly influences the reactivity in the NTC region, therefore influences the transition from a cool flame to a hot flame. Further investigations determining the rate constants of the reactions of the $CH_3OCH_2$ radical may be needed to improve the DME ignition kinetics.