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Study on pressure dependences of ethanol oxidation by separated weak flames in a micro flow reactor with a controlled temperature profile

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Abstract

Detailed oxidation process of a stoichiometric ethanol/air mixture and its pressure dependence were examined based on separated weak flames in a micro flow reactor with a controlled temperature profile. With the increase of pressure, the first weak flame, which is stabilized at the lower temperature side, shifted to the low temperature side, and the peak value of its luminosity increased. The peak value of luminosity at the second weak flame, which is stabilized at the higher temperature side, increased from $P = 1$ to 2 atm, then decreased from $P = 2$ to 5 atm. Pressure dependences of the computed heat release rate (HRR) profiles with detailed ethanol mechanism developed by Saxena and Williams (UCSD mechanism) agreed with those of the experimental luminosity profiles. The contributions of elementary reactions to the peak values of HRR at the separated weak flames were investigated. Results showed that the first weak flame was characterized by the oxidation from the fuel to CO and the second weak flame was characterized by the CO oxidation and hydrogen-oxygen reactions. Reaction path analysis was conducted and the HO_2 formation reaction, $H + O_2(+M) \Longleftrightarrow HO_2(+M)$, CH_3CHO oxidation reactions, and reactions between C_2H_4 and C_2H_5 showed main pressure dependences at the first weak flame. Computation with Marinov's mechanism (LLNL mechanism) was conducted and pressure dependences of the HRR profiles did not agree with those obtained with UCSD mechanism, although pressure dependences of mass burning velocities and ignition delay times by these two mechanisms agreed well. The difference in the pressure dependences of the HRR profiles by these two mechanisms would be mainly due to the different pressure dependence of the HO_2 formation reaction. The increase of reactivity at the first weak flame in elevated pressure condition was overestimated in UCSD mechanism, while it was underestimated in LLNL mechanism.

Keywords: Microcombustion; Ethanol oxidation; Hydroperoxyl radical (HO_2); Pressure dependence; Weak flames

1. Introduction

Ethanol is one of the promising biofuels and its reliable kinetic model is required for the development of future efficient combustion devices. A number of kinetic models for ethanol have been developed [1–5] and predicted combustion characteristics by those models have been compared with various experimental results such as laminar burning velocities [1,3,6–9], ignition delay times [1,3,5,7,10], and species profiles in flow reactor [3,4,7,11], jet-stirred reactor

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