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Numerical Study on the Activated Chemical Species Governing Auto-Ignition of an Ethanol Spray

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Abstract

This study deals with the development of controlled-ignition technology for high performance CI (Compression Ignition) alcohol engines. Ignition control is the key technology for the development of such CI alcohol engines. Among the alcohol fuels, we focused on Ethanol as a promising candidate of alternative fuels replacing from petroleum. The objective of this study is to physically and chemically reveal the mixture formation process up to auto-ignition of an Ethanol spray. In our previous theoretical and experimental studies, reason of poor auto-ignition quality of an Ethanol spray was revealed. That is the difficulty of simultaneous attainments of auto-ignition suitable mixture concentration and temperature in an Ethanol spray formed by fuel injection due to its smaller stoichiometric air/fuel ratio and much greater heat of evaporation compared with conventional diesel fuel. In addition, this knowledge was also confirmed by numerical analysis with the investigation of spatial distributions of mixture concentration and temperature and their temporal histories from fuel injection. Based on those studies, required surrounding gas conditions for stable auto-ignition was physically cleared. However, chemical mechanism of Ethanol auto-ignition is still at question. Therefore, as the next step, it was numerically investigated that auto-ignition of an Ethanol spray is dominated by what kind of activated chemical species created in its mixture formation process. One of the commercial CFD codes; CONVERGE was used in the computational calculation with the considerations of turbulence, atomization, evaporation and detailed chemical reactions. We focused on the molar fraction of activated chemical species such as OH and H at the location where auto-ignition occurred within an Ethanol spray. Required physical and chemical conditions for auto-ignition of an Ethanol spray and their simultaneous attainment during mixture formation process are mainly discussed in this paper.

Keywords*:* Ethanol spray, Mixture Formation, Auto-Ignition, Numerical Analysis, Chemical species