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CFD Analysis of OME Spray Combustion

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To stop global warming and achieve carbon neutrality by 2050, e-fuels, produced from CO_2 and H_2 using renewable energy sources, are attracting attention. Among them, polyoxymethylene dimethyl ethers are promising alternative fuels for compression ignition engines. Polyoxymethylene dimethyl ethers are a class of ethers with the molecular structure $CH_3(\text{-O-}CH_2)n\text{-O-}CH_3$, called OMEn. OMEn n>2 are liquid at room temperature and pressure, exhibiting good ignitibility and low soot formation properties. However, the physical properties of OME are different from diesel fuel. It is necessary to understand the spray combustion behavior for optimization of the fueling system, because spray characteristics play an important role in direct injection compression ignition engines.

In this paper, the spray and combustion characteristics of OME_3 were investigated using numerical simulation with a chemical kinetic mechanism. High speed observation of OME_3 spray was made in a constant volume vessel under an engine-relevant ambient condition, and numerical simulations are validated via the experimental data.

CONVERGE CFD software version 3.0 was used to perform spray simulation. Sprays are modeled using a modified KH-RT breakup and LES turbulence models. Fuel injection rates are specified based on measured data. A reduced 76 species 273 elementary chemical kinetic mechanism of OME_3 developed by Sakai on the basis of detailed mechanism of Cai was used for chemical reaction. Figure 1 shows the comparison of numerical calculation results of OME_3 non-reacting spray penetration length with experiments. The calculation results give good agreement with the experiments for both the vapor and liquid penetration. Figure 2 shows the images of reacting spray of OME_3 and diesel fuel obtained from experiments and calculated distributions of temperature, equivalence ratio, intermediate products of CO, CH_2O and NO at 1.0 msec after start of injection. The equivalence ratios inside OME_3 spray are much smaller than diesel fuel because OME_3 has oxygen in its molecule and the stoichiometric air/fuel ratio is small. Therefore, there are more higher temperature area in OME_3 spray, and CO and NO are formed earlier than diesel fuel. Higher concentration of CH_2O is formed near the center of OME_3 spray, which suggests the low temperature oxidation proceeds inside the spray.

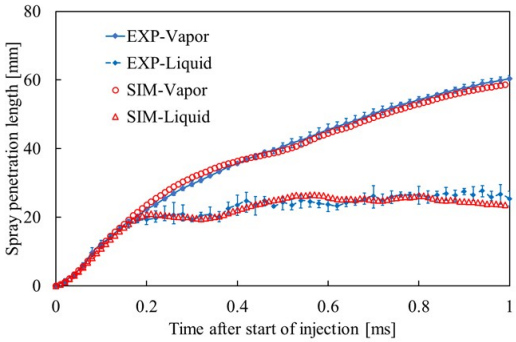

Fig.1 Comparison of numerical calculation results of OME_3 spray penetration length and liquid length with experimental ones

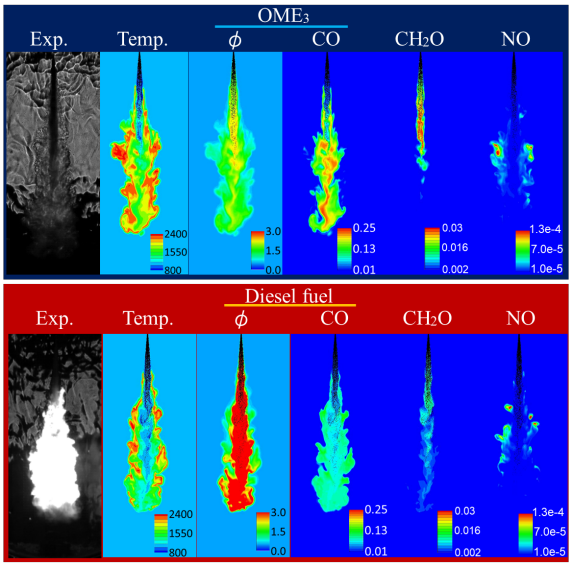

Fig.2 Experimental and numerical calculation results of spray combustion of OME_3 and diesel fuel at 1.0 msec after start of injection