

Construction of a Chemical Kinetic Mechanisms for Carbon Neutral Fuels (MtG: Methanol to Gasoline, EtG: Ethanol to Gasoline) in Spark-Ignition Engines

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For addressing global warming, there is a strong call for the automotive industry to achieve carbon neutrality. E-fuel is the one way to reduce the exhaust amount of greenhouse gases that can be used for existing automobiles and infrastructure. In this study, the combustion characteristics of Methanol to Gasoline (MtG), Ethanol to Gasoline (EtG) and commercial gasoline fuels were elucidated by measuring laminar burning velocities in constant volume combustion vessel. Additionally, a chemical kinetic reaction model capable of accounting for full PIONA compositions (Paraffins, Iso-paraffins, Olefins, Napthenes, Aromatics) was developed using ANSYS CHEMKIN-Pro to accommodate synthetic fuels and biofuels. To reproduce the compositional differences among gasoline, MtG, and EtG, a six-component surrogate chemical kinetic model was constructed. This model was built upon the oxidation mechanisms of gasoline surrogate components and detailed aromatic reactions proposed by Cheng et al. and Kalvakala et al., initially incorporating five components: isooctane, n-heptane, pentene, and trimethylbenzene. Furthermore, the detailed toluene reaction mechanism from Miyoshi et al. was integrated to complete the six-component surrogate chemical reaction model.

To evaluate the laminar burning velocity of real fuels and its sensitivity to the equivalence ratio, flame propagation visualization experiments were performed using the constant volume combustion vessel. The experiments were conducted under constant initial conditions of an initial pressure of 300 kPa and an initial temperature of 423 K, with the equivalence ratio (ϕ) varied from 0.9 to 1.4 in increments of 0.1. The experimental results demonstrated that three fuels exhibited similar equivalence ratio dependencies, with the laminar burning velocity reaching a maximum near an equivalence ratio $\phi=1.1$. In the lean combustion region ($\phi \leq 1.0$), no significant differences in laminar burning velocity were observed among three fuels. The laminar burning velocity in the rich combustion region ($\phi \geq 1.1$) decreased in the order of Gasoline, EtG, and MtG.

Model reduction was subsequently carried out using the DRGEPSA method, yielding a reduced reaction mechanism consisting of 183 chemical species and 951 elementary reactions. The sampling points for the reduction process were designated over specific pressure, temperature, and equivalence ratio ranges representative of internal engine cylinder conditions. Calculation and analysis results of the adiabatic flame temperatures revealed distinct behavior depending on the mixture stoichiometry. In the lean region, gasoline exhibited higher adiabatic flame temperatures compared to MtG and EtG. Conversely, under rich conditions, both MtG and EtG achieved adiabatic flame temperatures equivalent to that of gasoline. This disparity among fuel types is primarily attributed to the higher proportion of low-reactivity components, such as isoparaffin and aromatics, present in MtG and EtG, which contributed to the reduced adiabatic flame temperatures in lean mixtures.

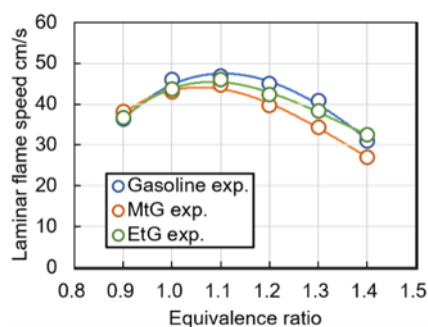


Fig.1 Variation of laminar flame speed with different fuels
(Initial pressure: 0.3 MPa, Initial temperature: 423 K,
equivalence ratio: 0.9~1.4)

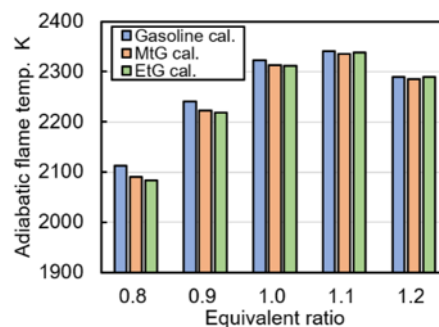


Fig.2 Changes in toluene consumption rate during
the combustion process of each fuel