Determining the Potential of Light Naphtha as Novel Alternative Fuel Using Predictive Kinetic Models

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Global energy demand is rapidly growing, primarily from developing countries, and conventional fuels continue to dominate our energy infrastructure. Global warming and pollutant emissions are major concerns. This research focuses on exploring alternative fuel options for diversification and use in future high-efficiency low-emission engines. This novel study conducted and developed predictive kinetic models for a targeted alternative fuel, light naphtha. The reactivity of light naphtha was analyzed by measuring ignition delay times in a shock tube which is an ideal reactor for kinetic studies. The measured data helped formulate a Primary Reference Fuel surrogate for light naphtha, which is needed for future high-fidelity computational fluid dynamic (CFD) simulations of an engine. The ignition delay experiments were conducted over a range of pressures, temperatures and equivalence ratios. The ignition delay times can be divided into three regions; high temperature (HTC), negative temperature coefficient (NTC) and low temperature (LTC) regions. In the HTC and LTC regions, ignition delay times increased as temperature decreased. This can be attributed to the exponential scaling of ignition delay time with the inverse of temperature. In the NTC region, ignition delay times show unexpected trend of decreasing reactivity with increasing temperature. In conclusion, a mixture of n-heptane and iso-octane is found to work well as the surrogate for light naphtha. This validated kinetic mechanism can be used in future CFD simulations for predictive optimized design of engines and turbines. Future engine experiments with light naphtha will be performed to optimize the design for high-efficiency and low-emission performance.