

Contribution of alternate PAH production routes in transportation fuels combustion

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Abstract

To better control Polycyclic Aromatic Hydrocarbons (PAH) emission and minimize their health and environmental effects, it is crucial to better understand their formation mechanisms. In the present work, we developed a new detailed chemical kinetic mechanism describing accurately both low- and high-temperature ignition and combustion of a wide range of automotive and aviation fuels as well as the formation of PAH up to coronene, suspected to be major soot precursors. Surrogate mixtures containing n-decane, iso-octane and n-propylbenzene were selected to represent the above mentioned fuels based on their cetane numbers and threshold sooting index. Including new reactions paths from recent studies [1,2] resulted in the improvement of mechanism predictivity over a wide range of experimental conditions (shock tubes, jet stirred reactor, burner stabilized premixed flames, and freely propagating premixed flames). The mechanism is able to reproduce PAH mole fraction profiles for a variety of fuels ranging from methane to Diesel fuel. The present study also shows that the chemical kinetic mechanism developed can be employed to predict combustion of jet-A1 and diesel fuels.

Following the mechanism validation, reactions path analyses were performed to identify PAH formation pathways from laboratory fuels (e.g. ethylene) to liquid transportation fuels oxidation (e.g. jet-A1 fuel). The impact of the fuel structure and reaction progress (e.g. height above the burner) on the respective importance of benzene and naphthalene formation reaction routes were also characterized, highlighting the contrasted contributions of phenyl + vinylacetylene and benzyl + propargyl steps. In line with recent experimental findings [3], a path involving dibenzofuran was found to play a key role in naphthalene production in jet-A1 flame, indicating a significant involvement of such species in PAH production in middle distillate combustion.

Key Words: Liquid Transportation Fuels; Surrogate; Chemical kinetic mechanism; PAH; Modeling

References

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