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Investigation on Combustion Chemistry of Aromatic Hydrocarbons Using Synchrotron and Kinetic Modeling Tools

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Aromatic hydrocarbons are a major component family in petroleum-based transportation fuels and their surrogate fuels, and are also key precursors of soot. The benzene ring structures of aromatic hydrocarbons result in complex intermediate pools in their combustion, especially the great amount of large free radicals and isomers, making aromatics combustion one of the most complicated targets for combustion diagnostics. In recent years, synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS) has been introduced to investigate pyrolysis and flame chemistry of aromatic hydrocarbons. The unique simultaneous detectability of SVUV-PIMS for free radicals and isomers help detect a variety of free radicals and distinguish a great deal of isomers. The mole fraction profiles of combustion species were measured as the function of heating temperature in the flow reactor pyrolysis and the function of distance from burner surface in the premixed flames, providing useful validation data for kinetic models of aromatics combustion. Based on recent theoretical progresses in combustion kinetics of aromatic hydrocarbons, kinetic models of benzene, toluene, styrene, ethylbenzene, o-xylene, n-propylbenzene and tetralin combustion have been developed and validated against both our SVUV-PIMS data and previous experimental data. For example, the vast amount of validation data of the toluene model include species profiles in flow reactor pyrolysis and oxidation, shock tube pyrolysis and oxidation, jet stirred reactor oxidation and premixed flames, and global combustion parameters such as ignition delay times and laminar flame speeds, covering a wide range of conditions from low to high temperatures, subatmospheric to high pressures and very lean to pyrolysis conditions. The decomposition kinetics of aromatic hydrocarbons investigated and the formation kinetics of PAHs were investigated using modeling tools such as the rate of production analysis and sensitivity analysis.

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