596e Methodology for the Simulation of Complex Hydrocarbon Mixtures

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Most transportation fuels involve complex hydrocarbon mixtures of normal paraffins, cyclo- and branched paraffins, aromatics and sometimes even olefins. These mixtures commonly involve hundreds of compounds, and the species concentrations can vary depending on the crude source and the processing methods at a given refinery.

There is considerable interest in performing computer simulations of the combustion and pollutant formation behavior of common transportation fuels such as jet fuel, diesel and gasoline. In order to perform such detailed simulations, a simplified characterization of the fuel is often needed. This presentation outlines a methodology for the formulation of fuel surrogates to be used in computational efforts, as well as experimental validation. Although the approach is demonstrated here as applied to common petrochemical distillate fuels, the methodology described is equally applicable to the range of new alternative fuels resulting from various gasification and indirect- and direct-liquefaction processes.

The approach involves the use of group contribution methods to represent the structural contributions of the various fuel components to the physical and chemical properties of the fuel. The forcing functions for the determination of specific compounds and concentrations to be used are obtained from: 1) an evaluation of key physical and chemical properties pertinent to the particular application of the fuel; 2) availability of kinetic parameters for the surrogate species under consideration; and 3) a cost and availability analysis for the surrogate species if experimental validation will be performed.

A case study using jet fuel (JP-8) will be presented that will provide an illustration of how a surrogate fuel can be developed, validated, and then used in detailed simulations of jet fuel droplet combustion. In order to accurately simulate the jet fuel or surrogate behavior, a detailed chemical kinetic mechanism was developed that is capable of describing the combustion and soot precursor chemistry relevant for the intended use. The mechanism was subsequently coupled with a CFD model (UNICORN) for simulations of fuel droplet evaporation and combustion in a laminar flow drop tube furnace, which was configured to mimic combustion behavior in a modern gas turbine.