Analysis of Hydrocarbon Fuels by NMR Spectroscopy:
Applicability to the Development of Fuel Surrogates and Thermophysical Models

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The analysis of hydrocarbon fuels by ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectroscopy will be discussed. NMR spectroscopy is particularly useful for the analysis of complex hydrocarbon mixtures for two reasons. First, several important structural moieties (such as olefins or aromatics) are segregated into specific spectral regions. Second, spectra can be collected in such a way that the spectrometer is equally sensitive to all ^{13}C nuclei (or to all ^{1}H nuclei). As a result of these two features, NMR spectroscopy readily provides the mole fractions of various classes of hydrocarbons (such as aromatics and linear alkanes) in a sample without the need to calibrate. NMR spectroscopy also gives easy access to other average properties for the components of each fuel sample, such as the extent and type of alkane branching. Such information is useful for the development of realistic fuel surrogates and reliable thermophysical models. The advantages and disadvantages of NMR spectroscopy will be illustrated by spectral analyses for two types of fuel samples: gas turbine fuels (i.e., jet fuel) and hydrotreated renewable diesel fuel. A discussion of sources of uncertainty in such an analysis will be included. Finally, a comparison of the results obtained by NMR spectroscopy to analyses by GC-MS and GC-FID will be discussed.