Thermophysical and Thermochemical Surrogate Mixtures for Gasoline Fuels

Ahfaz Ahmed [S], William L. Roberts and S. Mani Sarathy [C]
Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Mecca, Saudi Arabia
Mani.Sarathy@kaust.edu.sa

Transportation fuels are complex mixtures of numerous compounds, which makes them challenging to study experimentally and computationally. Thus, surrogate fuels having a smaller number of constituents are prepared with similar physical and chemical properties to enable computational simulations. Surrogate fuel modeling for transportation fuels opens a wide window of prospects for designing fuels to obtain higher efficiency and lower emissions. Ideally a surrogate fuel should be tailored to encompass all pertinent physical and chemical aspects of the real fuel to accurately mimic its combustion performance. While formulating surrogate blends, certain target properties of the real fuel are selected based on their relevance towards intended applications. This approach has proven to be decisive while studying new fuels for which combustors are yet to be optimized. The present work introduces thermophysical and thermochemical surrogate mixtures of several gasoline fuels. The surrogates are formulated using a computational model with property simulations and a regression algorithm to find optimal surrogates matching a range of target properties. The target fuels include six FACE (**F**uel for **A**dvanced **C**ombustion **E**ngines) gasolines and two certification gasolines. The target properties include hydrogen/carbon (H/C) ratio, density, distillation characteristics, carbon types, heat capacity, enthalpy of formation, enthalpy of combustion, and entropy of formation. The results of simulations and experiments are presented to validate the surrogate fuels