Consistent Prediction of Thermodynamic Properties for Sustainable Aviation Fuel Components

Eugene Paulechka[1, S, C], Andrei Kazakov[1], Chris Muzny[1], Suphat Watanasiri[2] and Abhijit Dutta[2]

[1]*Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, CO, U.S.A.*
[2]*Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, U.S.A.*
yauheni.paulechka@nist.gov

Air transportation is one of the main sources of greenhouse gases. Production and use of sustainable aviation fuels (SAF) is one of the promising measures explored to constrain this negative impact.

Both alternative and fossil jet fuels are composed of aliphatic, alicyclic (mono-, bi-, and tricyclic), and aromatic hydrocarbons. The hydrocarbon composition of the fuels can be very different. The specifications are primarily based on the fuel performance. Distillation temperatures, density, flash point, and net heat of combustion are included in the fuel specifications. The use of composition-based predictions of these properties can help expedite the evaluation of potential candidates and guide the development of SAF. Thermodynamic properties of pure components including normal boiling temperature, enthalpy of formation, enthalpy of vaporization, and density are required as input for these methods. In this work, evaluation of the experimental data and prediction for these properties are considered. The fuel components belong to different homologous series and the property consistency within a series are used to improve the available experimental or predicted values.

Out of all considered properties, the high-level ab initio calculations are available for the gas-phase enthalpy of formation. For the compounds with no experimental data, the values obtained with the local CCSD(T)/QZ protocol [1] were preferred. For many compounds, for example, di- and trisubstituted cyclohexanes, the group-contribution predictions were found to be unsatisfactory. For long-chain homologues, the ab initio value for the short-chain base structure was combined with an empirical CH_2 increment. With the group-contribution methods, density (molar volume) and enthalpy of vaporization could be reasonably predicted for some homologous series. A more efficient approach included a combination of a reliable experimental property value for a base structure with a corresponding increment. This methodology, together with the Riazi-type correlations, was also successfully used for normal boiling temperature.

References

1. Paulechka and Kazakov. J. Chem. Theor. Comput. 2018, 14, 5920.