Combined machine learning techniques to predict the thermal conductivity of liquid mixtures

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Abstract:

Mitigating climate change caused by global warming requires a significant reduction in greenhouse gas emissions, particularly carbon dioxide. In the context of aviation transport, the development and use of sustainable aviation fuels (SAFs) is one of the pathways seriously considered to reduce CO_2 emissions. Various biomass conversion processes involve high pressure and temperature conditions, and the design and dimensioning of such processes require thermophysical property data, particularly the thermal conductivity (λ). Moreover, in aircraft thermal management systems, the fuel itself acts as an internal heat sink, and it is therefore important to anticipate during the design of a fuel, the impact of the fuel's composition on its thermal properties, making λ one of the key properties for jet fuels. Although new experimental devices have been proposed to reduce time, costs and product consumption [1], available λ values for fluids remain scarce and the need of predictive models is of the utmost importance.

This communication focuses on the application of Machine Learning-based techniques to develop a fully predictive framework for estimating the thermal conductivity of multi-component mixtures containing hydrocarbons and oxygenated compounds. The work was performed in three steps: (i) quantitative structure-property relationship (QSPR) models were developed to predict the thermal conductivity of pure compounds [2,3], (ii) symbolic regression was then applied to generate mixing rules on the basis of a database containing binary mixtures for which compositions and λ values of mixtures and their components are experimentally known, (iii) a mixing rule has been designed for the case of multi-components (three and more) mixtures, and QSPR models were used to power mixing rules to predict the thermal conductivity values of complex mixtures [3].

The fully predictive methodology was finally applied to predict the thermal conductivity of four jet fuel samples at different temperatures and atmospheric pressures, resulting in a mean absolute error of 2.9%. Performed comparisons confirmed the relevancy of the developed methodology, effective for a wide range of hydrocarbons and oxygenated compounds mixtures.

Bibliography :

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