

Mixture-QSPR for Sustainable Aviation Fuels: Predicting Non-Linear Effects in Oxidation Stability

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The decarbonization of aviation transport relies primarily on Sustainable Aviation Fuels (SAFs), which, to be deployed, must comply with strict international specifications in terms of composition and physicochemical properties^[1]. As SAFs consist of complex hydrocarbon mixtures, understanding and predicting the behavior of their properties remains challenging, particularly due to the presence of non-linear mixing effects in several properties^[2]. Oxidation stability, which is a key fuel property, was investigated in this work through combined experimental measurements and modeling approaches. A database including experimental Induction Period (IP) values, an indicator of oxidation stability, was assembled and currently contains 325 IP values for single compounds and 163 for binary mixtures representative of jet-fuel hydrocarbons. This database was used to develop Mixture Quantitative Structure-Property Relationship (M-QSPR) models. As M-QSPR remains significantly less established than single-compound QSPR^[3], the identification of relevant descriptors capable of encoding mixture information is still a key challenge. Several combinations of molecular and mixture descriptors were systematically evaluated. We report predictive models of the IP based on the composition of the mixture and using recently derived physico-chemical ingredient descriptors^[4]. These models achieved external Q^2 values of 0.843, 0.837, 0.741, and 0.677 under progressively more stringent external validation strategies (Points-Out, Mixtures-Out, Compounds-Out, and Everything-Out, respectively).

Bibliography :

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