Choice of a kerosene surrogate for prediction of the emission of carcinogenic polycyclic aromatic hydrocarbons

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The component composition of kerosene is very complex and depends on the brand, feedstock and manufacturer, for this reason, model fuels are used in calculations - surrogates consisting of several well-studied substances. The paper validated 14 surrogates of aviation kerosene, which can be used to predict the emission of carcinogenic polycyclic aromatic hydrocarbons (PAH) using the kinetic model of the Samara University "A17". The surrogates were verified using experimental data for normal flame propagation velocity, low-temperature pyrolysis, and combustion of pre-evaporated kerosene. The obtained results show the significance of reproduction of molar mass and carbon number by surrogates. The use of trimethylbenzene, methylnaphthalene, tetralin and xylene isomers in surrogates contributes to a better description of the low-temperature oxidation of kerosene aromatic compounds. Predicting the concentrations of combustion products showed that the Liu and Drexel surrogates describe the concentrations in the front better than others, but the concentrations of the equilibrium products can be overestimated. Surrogates UM1 and su4 more accurately predict concentrations in the post-flame zone. As a result of the review, the su4 surrogate was chosen for use in future computational work in the region of high and low temperatures.