

An Experimental and Numerical Study of Combustion Chemistry of Fatty Acids Esters

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Depletion of petroleum sources makes search for alternative fuels quite relevant. Biodiesel based on methyl and ethyl esters is one of the most promising types of oxygenated fuels. CFD methods are used to optimize the construction and increase the efficiency of engines. Knowledge of the kinetic mechanisms for combustion of biodiesel fuels is necessary to use this method. One of the most informative techniques for studying combustion chemistry is probing molecular-beam mass spectrometry (MBMS), which in combination with numerical simulation makes it possible to develop and validate the combustion mechanisms for biodiesel combustion.

The aim of this work includes obtaining new experimental and modeling data on the structure of flame of model biodiesel fuels, among them methyl acetate (EA), ethyl butanoate (EB), ethyl pentanoate (EP), methyl propanoate (MP), methyl hexanoate (MH) as well as blends of MH or EP with n-heptane/toluene mixtures.

The flames of blends of the above listed fuels with oxygen and argon were stabilized on a flat burner at atmospheric and subatmospheric pressures. Microthermocouples and MBMS with soft ionization by electron impact and VUV photoionization were used for measuring the temperature and mole fraction profiles of reagents, the main combustion products and intermediate species, including unsaturated hydrocarbons, which are known as potential soot precursors. In total more than 30 intermediate species were identified in the studied flames and their mole fraction profiles, including atoms and radicals, were measured quantitatively. The experimentally measured mole fraction profiles of species were compared with the modeling results, obtained using mechanisms developed earlier. It was established that the used mechanisms quantitatively predict the mole fraction profiles of the main initial reagents and final combustion products, but for most intermediate species the agreement between the results of modeling and measurements is basically of a qualitative nature. These discrepancies indicate the need for further improvement of the tested kinetic mechanisms. The analysis of the primary reaction pathways for isomeric esters (EA – MP, EB – MP, EP – MH) showed that for ethyl esters reactions of monomolecular decomposition produce ethylene and the corresponding fatty acids while for methyl esters the key transformations occur via interactions with H, OH and O. It is established that the contribution of monomolecular decomposition reactions of ethyl esters is noticeably increased with increasing fuel-air equivalence ratio.