Effects of the unsaturation degree in methyl esters on the combustion process

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Different approaches have been developed to reduce the dependence on fossil fuels. A successful strategy in transportation is the use of biofuels, such as biodiesel or bioethanol. These are easy to implement and to produce at large scale. Different studies have been carried out with the aim to understand the potential of biofuels to reduce the emission of regulated pollutants, such as NOx, soot, and HC. A significant number of studies have been performed either using a mixture of biodiesel and diesel fuel in engines, or individual fuel in laboratory combustion devices including jet stirred reactors and opposed flow diffusion flames. However, studies that aim at understanding the combined reaction pathways of such fuel mixtures remain scarce. Here, we report an investigation of the joint combustion processes of prototypical ester fuels and hydrocarbons to characterize the chemical changes induced by the oxygenated fuels in low-pressure premixed flames.

We have chosen ethene as a well-studied base fuel, and we have added two C4 methyl esters: methyl butanoate (MB) and methyl crotonate (MC), with a different unsaturation degree. The unsaturation degree has a significant impact on several properties of the fatty acid methyl esters (FAME) present in the biodiesel currently used in engines. For this reason, a set of five fuel-rich ($\phi=1.6$) laminar premixed flames at 40 mbar of MC, MB, and ethene as well as mixtures of ethene and the corresponding methyl ester were investigated using electron ionization molecular beam mass spectrometry (EI-MBMS). In this series of flames, the equivalence ratio, argon dilution, pressure, and gas velocity were kept constant.

Special attention was given to identify potentially undesirable compounds. The methyl esters promote the formation of oxygenated species, for example CH$_3$COOH, C$_3$H$_4$O, and C$_3$H$_6$O, but no clear tendency as a function of the unsaturation degree was observed. Furthermore, the mole fraction of acetylene produced in the flame is independent of the fuel structure. A higher production of soot precursors was observed in MC flames. For instance, C3 species associated with propargyl or allyl radicals are the main soot precursors observed in the MC flames. The benzene mole fraction is higher in MC than in MB flames; it is probably produced by the propargyl recombination reaction. If the dilution effect of the MC is taken into account in the ethene - MC flames, an increase in the C$_3$H$_5$ species is observed evidencing the interaction between MC and ethene to produce different soot precursors. Therefore, the results suggest that a reduction of polycyclic aromatic hydrocarbons (PAH) and soot precursor formation can depend sensitively on the kind of the unsaturated species present in the initial fuel mixture.