Molecular beam mass spectrometric study of the laminar flame structure of ethyl levulinate

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4-oxopentanoic acid ethyl ester or just ethyl levulinate (EL) is considered as one of perspective fuels from cellulosic biomass. It could be easily derived from inexpensive woody biomass with a high yields [1] making this biofuel especially attractive. In different works EL is considered either as a diesel additive [1,2] or as an octane booster [3,4]. Such ambiguity stems mainly from the lack of kinetic studies of EL. Although levulinic fuels have become popular in the last five years, only a few kinetic studies on EL reactivity are presented in literature. Therefore this study aims to broaden the experimental database on this fuel along with validation of existing kinetic conceptions.

Fuel-rich (φ=1.4) laminar premixed flame of EL/O_2/Ar mixture was chosen as the main object. The flame was stabilized over a flat flame burner at atmospheric pressure. Chemical speciation in the flame front was measured via the molecular-beam mass-spectrometric technic. The reactants, stable and intermediate products including the main flame radicals were detected.

Since EL has both ester and ketone functionalities, the measurements were focused on the specific intermediates such as levulinic acid and methyl vinyl ketone to track the corresponding reaction pathways. The work of Ghosh et al.[4] was used as the basic kinetic scheme for the analysis. The results obtained have shown the peculiarities of the competition between the esteric and ketone pathways.

References

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