Study of cation chemistry in ethylene flames

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The flame is a weakly ionized plasma. Understanding the ion chemistry in a flame is crucial for the development of new diagnostic methods, as well as for the development of ion-sensitive technologies for controlling combustion processes. In this work, the spatial distribution of positive ions (cationic structure) in premixed ethylene/oxygen/argon flames stabilized on a flat-flame burner at atmospheric pressure was measured by molecular beam mass spectrometry in a wide range of equivalence ratios ϕ = 0.4÷1.5. Numerical calculations of the cationic structure of these flames as well as profiles of the rate of production of the main flame ions have been carried out using the Cantera software (V.2.5.1) [1]. For the calculations, a detailed ion chemistry mechanism was used. The mechanism was developed on the basis of ion chemistry models available in the literature [2] and augmented with reactions for the $C_3H_5^+$ cation. A comparison of the experimental and simulation data has shown that the mechanism correctly describes the relative content of the most abundant oxygen-containing cations (CH_5O^+, $C_2H_3O^+$) in flames, as well as of the $C_3H_5^+$ cation found experimentally in a rich flame (ϕ=1.5). However, the mechanism significantly underestimates the relative mole fraction of the $C_3H_3^+$, a key cation in fuel-rich flames. Several aromatic and cyclic cations with the general formula C_xH_y were also detected in the fuel-rich flame (ϕ=1.5). The obtained data will serve as a basis for further improvement of the ion chemistry mechanism in fuel-rich hydrocarbon flames.

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References

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