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Kinetic Modeling of Low-Temperature Plasma Assisted Combustion

IGOR ADAMOVICH, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43210

Quantitative insight into kinetics of low-temperature plasma assisted fuel oxidation and ignition would be impossible without kinetic modeling. The principal challenges in development of a predictive kinetic model of nonequilibrium plasmas sustained in fuel-air mixtures include (i) lack of "conventional" chemical kinetics mechanisms validated at low temperatures, (ii) lack of data on rates and products of reactions of excited species generated in the plasma, some of which are not well understood, and their coupling with fuel-air plasma chemistry, and (iii) scarcity of data obtained in well-characterized plasma-assisted combustion experiments, which can be used for model validation. "Conventional" combustion chemistry mechanisms have been developed for relatively high temperature conditions. Their applicability at temperatures below ignition temperature, common in plasma assisted combustion environments, needs to be assessed to determine if they can be used as a basis for a plasma-assisted combustion chemistry mechanism. This requires time-resolved measurements of radical species concentrations during low-temperature fuel oxidation, when an initial pool of primary radicals (O, H, and OH) is generated in the plasma. such as in the late afterglow of an electric discharge. This allows isolating relatively slow "conventional" low-temperature fuel oxidation reactions triggered by the radicals from the reactions of excited species generated in the discharge, which decay relatively rapidly. Kinetic modeling calculations demonstrated that some of the existing combustion mechanisms provide good agreement with the experimental data taken in lean H₂-, CH₄-, and C₂H₄-air mixtures at low temperatures, while data taken in $C_{3}H_{8}$ -air are not reproduced by any of the mechanisms tested. A complementary approach is to focus on kinetics of "rapid" reactions of electronically and vibrationally excited species in the electric discharge, as well as oxygen dissociation by electron impact, and their effect on production of radicals in the early afterglow. These experiments provide key data on coupling of molecular energy transfer processes in the plasma with "conventional" chemical reactions. Time-resolved and spatially-resolved measurements of temperature, vibrational and electronic levels populations, and radical species concentrations are critical for characterization of the nonequilibrium reacting mixture at these conditions. Kinetic modeling of recent experiments in a diffuse filament, nanosecond pulse electric discharges in air suggest that the role of electronically excited N_2^* molecules on chemical reactions in the afterglow, such as NO generation reactions, has been significantly underestimated in the past. Further experiments in fuel-air mixtures are expected to provide additional data on the role of these excited species on low-temperature fuel-air chemistry.