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Ion Chemistry Model for Methane Combustion

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Ion chemistry models for combustion of hydrocarbon fuels are required in order to simulate the interaction of electric fields with flames e.g. in electric field combustion control and flame sensing by means of ionization probes. Therefore we compiled a reaction kinetic model describing chemo-ionization in methane combustion, charge transfer, and recombination. Starting point was the reaction mechanism of methane combustion of the Gas Research Institute GRImech 3.0 to be used in the Chemkin software package. This model was complemented by reactions describing the formation of HCO^+, H_3O^+, CH_3^+, $C_3H_3^+$, and electrons by chemo-ionization and charge transfer and the formation of O^- and O_2^- negative ions by electron attachment to O_2-molecules [1-2]. Implementation of this reaction mechanism into the PREMIX module of Chemkin 3.7 resulted in ionization degrees for premixed methane-air flames at atmospheric pressure having the correct order of magnitude. The concentration profiles of electrons and ions, however, were not realistic because Chemkin 3.7 did not take into account space charge induced electric field formation impeding diffusion induced charge separation on length scales exceeding the Debey length in the flame plasma [3]. Further we found that the chemistry solver has not the accuracy which would be required in order to simulate space charge densities correctly.

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[2] A.N. Eraslan, R.C. Brown, Combustion and Flame Vol. 74, 19-37 (1988)

[3] Jens Prager: Modeling and Simulation of Charged Species in Lean Methane-Oxygen Flames. Dissertation, Ruprecht-Karls-University Heidelberg (2005), 117 pp.