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Computational modeling of nanoparticle charging mechanism in a hydrocarbon flame PARTH SHAH, ALEXEI SAVELIEV, North Carolina State University — A model that describes the charging mechanism of a 20 nm nanoparticle introduced in a methane-air counterflow laminar diffusion flame was developed and analyzed. The detailed kinetic model considers the production of ions and electrons in a methane-air flame due to chemi-ionization, thermal ionization and charging due to diffusion. The chemi-ionization model considers a one-step reaction that produces ions and electrons in a flame in addition to the detailed neutral reaction mechanism. The model is analyzed to study the effects of temperature, total nanoparticle concentration and chemi-ionization on charge formation in nanoparticles as well as on ions and electrons. The results show that thermal ionization is more dominant at high temperatures whereas diffusion charging is important at low temperatures. High concentration of nanoparticles influences the gas-phase ion and electron concentration to a very significant level whereas low concentration has a negligible effect on the same.

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