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Simulation of Electron and Ion Transport in Methane-Air Counterflow Diffusion Flames[1] SANGKYU CHOI, FABRIZIO BISETTI, SUK HO CHUNG, King Abdullah University of Science and Technology, CLEAN COMBUSTION RESEARCH CENTER TEAM — The spatial distribution of charged species in a methane-air counterflow diffusion flame is simulated with a detailed ion chemistry. The electric field induced by the distribution of charged species is calculated and compared to that obtained invoking the ambipolar diffusion assumption. The two calculations showed identical profiles for charged species and electric field. The profiles of ion mole fractions show two peaks: one near the maximum temperature and a second peak on the oxidizer side. The major ions near the maximum temperature are electron, C_2H_3O+ and H_3O+. CHO_3- and H_3O+ contribute to the second peak. These profiles are quite different from those adopting a simplified three-step mechanism based solely on E-, CHO+ and H_3O+, which shows only a single peak. Reaction pathway analyses showed that near the flame region, the proton is transferred by the path of CHO+ $\rightarrow$ H_3O+ $\rightarrow$ C_2H_3O+ $\rightarrow$ CHO+ in a circulating manner. In the second peak, CHO_3- is produced though the pathway of E- $\rightarrow$ O- $\rightarrow$ OH- $\rightarrow$ CHO_3-. The sensitivity of the charged species profiles to transport properties is investigated, and it is found that the variation of charged species profiles near peak temperature is relatively small, while on the oxidizer side, it is quite sensitive to transport properties.

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