Simulation of ozone formation in an electric discharge in mixtures of methane with air

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We took a model of the discharge at an atmospheric pressure in air, described in detail in [1] as a basis for our discharge model. We implemented it to describe the characteristics of quasistationary [1], pulsed [2] and corona [3] discharges, as well as the transition from corona discharge to a glow [4] discharge in air at atmospheric pressure at room temperature. The processes involving the methane molecule and its derivatives were taken from [5].

The calculations were performed for atmospheric pressure and room temperature for air and its mixtures with methane. A pulsed-periodic electric discharge and its afterglow in a gas flow were investigated by the homogeneous model. The maximum specific energy input in the discharge was 50 J/g. In the case of air, the dependence of the ozone number density in the afterglow zone on the specific energy input is close to linear. The addition of methane leads to a several times decrease in the ozone number density. The dependence of the ozone number density on the specific energy input differs markedly from linear.

It is known that atomic oxygen is formed as a result of dissociation of oxygen molecules by plasma electrons and collisions of molecular oxygen with electronically excited nitrogen molecules. Analysis of simulation results showed that the main mechanisms leading to a decrease in ozone concentration are competition of quenching of electronic levels of molecular nitrogen by oxygen and methane molecules [6-7]. The process of dissociation of methane in the discharge leads to the formation of hydrogen atoms, which also leads to a decrease in the concentration of oxygen and ozone atoms as a result of chemical reactions.

References

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