Numerical simulation of chemical reactions induced by ionization waves propagation from an atmospheric pressure plasma jet

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Abstract: Two-dimensional numerical simulation is conducted focusing on the behavior of ionization wave propagating from a kHz-powered atmospheric pressure helium plasma jet operated in dry air. The ionization wave initiated in the discharge core region propagates to ambient air, which induce ionization and excitation of air components, such as N_2^+, O_2^+ and O even in the afterglow region.

1. Introduction

The plume of a kHz-driven atmospheric pressure plasma jet consists of the propagation of streamer-like ionization waves. Pioneering numerical works have been done to describe this phenomenon[1,2]. However, it remains difficult to simultaneously simulate the plasma core region, where rapid reactions such as breakdown occur, and the afterglow region, where mixing with the surrounding air greatly affects the relatively slow chemical reactions, because the model must take into account complex mechanisms such as photoionization and Penning ionization. In this work, we developed a two-dimensional numerical model of a He-based atmospheric pressure plasma jet[3] and simulated the ionization propagation phenomenon and the chemical reactions induced by it.

2. Modeling

A steady-state fluid distribution describing the helium jet ejection to ambient dry air is assumed to simulate the plasma dynamics. The dV/dt of the applied voltage is approximately 4.5×10^9 V/s, with a peak value of 6 kV. The drift-diffusion equation and Poisson's equation are considered for the plasma. Chemical species, He, He^+, $He(2^3S)$, $He(2^1S)$, He_2^*, He_2^+, N_2, N_2^*, N_2^+, O_2, O_2^*, O_2^+, O_2^-, O_3, O_3^-, O, $O(^1D)$, O^-, and electrons, are considered. The model includes 60 electron collision reactions, 15 chemical reactions and 19 surface reactions.

3. Results

Figure 1 shows the spatial distribution of the maximum values of number densities and reaction rates. The position 0, 20 and 35 mm indicate the edge of powered electrode, the exit (open end) of discharge tube and outer boundary of numerical domine, respectively. Figure 1(a) shows that the number densities of electrons, He^+, $He(2^3S)$, and He_2^* are between 10^{18} and 10^{20} m^{-3} inside the discharge tube. They increases to about 10^{20} m^{-3} within an approximately 5 mm from tube exit. Figure 1(c) shows that the ionization and excitation rates of helium atoms are significant even outside the tube , which is due to the ionization wave propagation. This leads the ionization ambient oxygen and nitrogen molecular and production of reactive species (atomic oxygen) as shown in Figure 1(b) and (d).

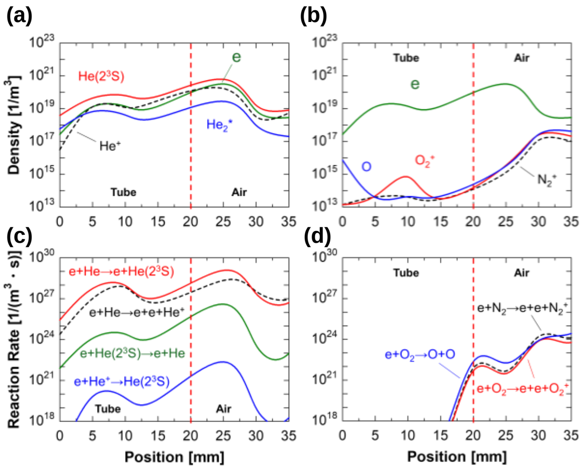

Fig. 1. Spatial distribution of species number densities (a, c) and reaction rates (b, d).

4. Conclusion

A two-dimensional reactive numerical simulation was conducted focusing on the behavior of ionization waves propagating from an atmospheric pressure helium plasma jet into surrounding air and the induced chemical reactions. The ionization wave initiated in the discharge core region propagates to ambient air, which induce ionization and excitation of air components, such as N_2^+, O_2^+, and O even in the afterglow region.

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