Formation of O and OH in atmospheric pressure He–air plasma jet

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Abstract: The dynamic behaviours of O and OH in APPJ sustained in He-air mixture and flowing into ambient air is studied. A two-dimensional neutral gas transport model and a plasma fluid model with a kinetic treatment of electrons are used. Production efficiency of O and OH, the critical production and destruction mechanisms, temporal-spatial evolution of O and OH concentrations during APPJ propagation, as well as interactions with substrate surfaces are presented. The dependences of O and OH densities on the controlling parameters are also analysed and discussed.

Keywords: atmospheric pressure plasma jet, reactive species, fluid model.

1. Introduction

The atmospheric pressure plasma jet (APPJ), as a sources of reactive species, has received considerable attention due to its efficacy in industrial, medical, and biomedical applications [1-2]. In these applications, reactive oxygen and nitrogen species play a major role. Understanding the production and delivery of these bio-active species in plasma jet is important to optimization jet plasma sources. In recent years, numerous experimental and numerical studies on this issue have been carried out [3-6]. The density, distribution, and production and loss processes of some reactive species in some APPJ system have been revealed. However, due to the complexity of plasma physics and chemistry in APPJ as well as the variety of geometries and discharge production techniques for APPJ [7-8], the understanding of the production and delivery of the reactive species in APPJ is still lacking. This paper focuses on the dynamic behaviours of O and OH in APPJ sustained in He-air mixture and flowing into ambient air.

2. Model

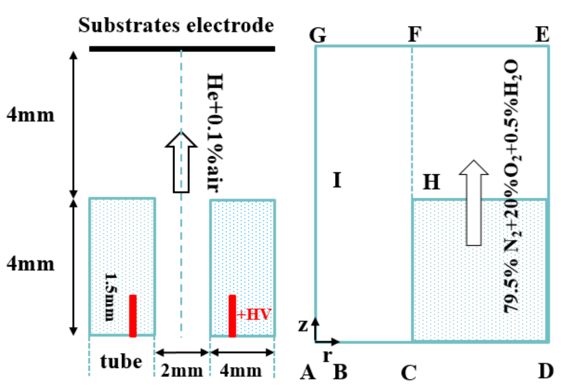

Fig.1 The jet configuration and computational domain

The plasma jet studied is generated in a dielectric tube with a ring electrode powered by a DC pulse. A substrates electrode is located 4 mm away from the tube exit. He+0.1%air working gas flows through the dielectric tube into ambient air. The simulation is based on a two-dimensional cylindrically symmetric model including two parts: neutral gas flow model and plasma dynamics model.

neutral gas flow model:

$$\nabla\cdot(\rho\boldsymbol{u})=0$$

$$\nabla\cdot(\rho\boldsymbol{uu})=-\nabla p-(\nabla\cdot\tau)+\boldsymbol{F}$$

$$\nabla\cdot(\rho\boldsymbol{u}w_i)+\nabla\cdot\boldsymbol{J}_i=0$$

Where u is the velocity vector of gas flow, ρ is the mixture density, τ is the stress tensor for a Newtonian fluid, respectively. J_i is flux for species i.

Plasma dynamics model:

$$\frac{\partial n_i}{\partial t}+\nabla\cdot\boldsymbol{\Gamma}_i=S_i$$

$$\boldsymbol{\Gamma}_i=\mathrm{sgn}(q_i)n_i\mu_i\boldsymbol{E}-D_i\nabla n_i+\boldsymbol{u}n_i$$

$$\frac{\partial(n_\varepsilon)}{\partial t}+\nabla\cdot\left(\frac{5}{3}\mu_e E n_\varepsilon-\frac{5}{3}D_e\nabla n_\varepsilon\right)$$

$$=-e\Gamma_e\cdot E-\sum_j\Delta E_j R_{inel,j}-3\frac{m_e}{M}k_b n_e\nu_{en}(T_e-T_g)$$

$$\varepsilon_0\nabla\cdot(\varepsilon_r\nabla\Phi)=-\sum_j q_i n_i$$

Where n, Γ and S are respectively the species density, flux and source term. q is the charge; μ and D are the mobility and diffusion coefficients, respectively; E is the electric field; Φ is the electric potential; T_e is the electron temperature; T_g is gas temperature. ΔE and R_{nel} are the energy loss during inelastic collisions and the corresponding reaction rate, respectively; m_e, M, and ν_{en} are the electron mass, ion mass, elastic collision frequency. ε_r is the relative permittivity of the dielectric and ε_0 is the vacuum permittivity.

The plasma chemistry used in this study consists of 29 species and corresponding 63 reactions. The reaction rate coefficients involving electron collision with heavy species and transport electron coefficients are calculated by a Boltzmann solver. Other rate coefficients come from references.

The above equation system is solved by a time-dependent solver of COMSOL and in simulation, the neutral gas flow model and plasma dynamics model are solved independently. The results of neutral gas flow model provide the background gas composition for the plasma dynamics model.

3. Results

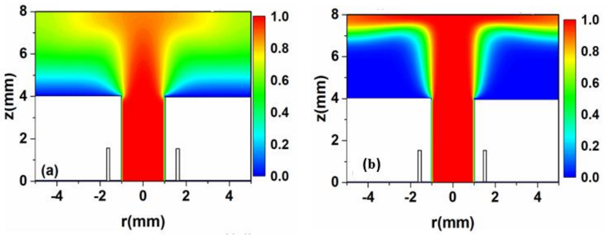

Fig.2 The helium mole fraction distribution under different gas flow rates: (a)1m/s, (b) 10m/s.

For different flow velocities, the helium mole fractions are almost 1 inside the tube. But away from the exit, He diffuses quickly along the radial direction and its mole fraction decreases fast in axial direction at lower flow rate. At flow rate of 10m/s, the radial diffusion of helium mole fraction mainly occurs near the substrate electrode.

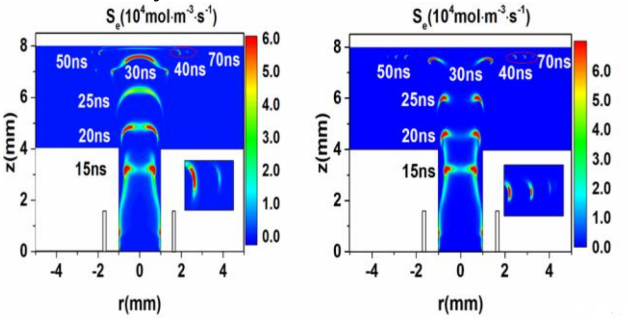

Fig.3 The ionization rate of the jet at different gas flow rates 1m/s (left) and 10m/s (right).

Before about 20 ns, under two flow rates, the ionization rate in the channel centre is lower and the plasma bullet has a ring shape. Afterwards, the ring-shape bullet changes into ball-like shape gradually, with the maximum ionization rate appearing in the channel centre for the lower flow rate. When the bullets under both flow rate reach the substrate a surface discharge occurs.

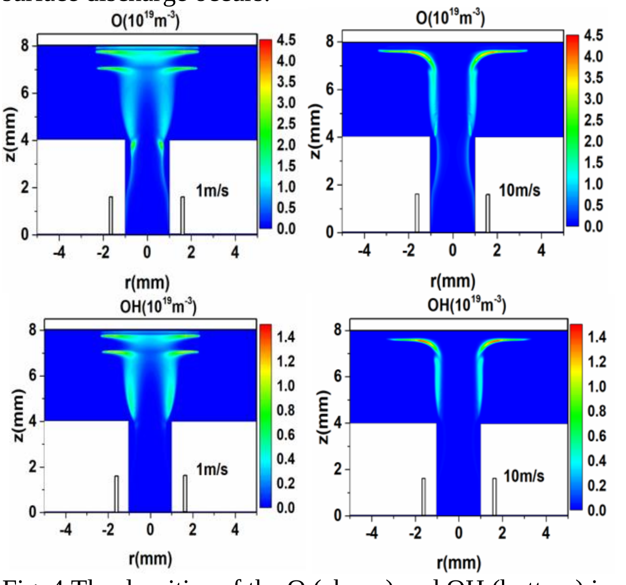

Fig. 4 The densities of the O (above) and OH (bottom) in different gas flow rate at 85ns.

O and OH are mainly generated outside the tube and the density in channel centre is lower than that on the outer surface of the He effluent, forming a donut-shaped distribution. At lower flow rate, the donut radius decreases with increasing the distance from the tube exit and on the surface of the substrate electrode, O and OH densities behave an approximately uniform distribution.

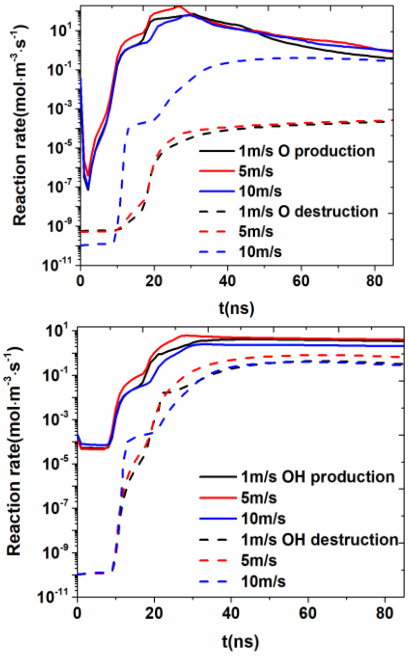

Fig.5 The time evolution of the reaction rate for the production and destruction of O and OH at different gas flow rate.

The highest O atom production rate is achieved at about 20 ns when the plasma jet leaves the nozzle. At high flow rate the destruction of O atom is serious, but the flow rate only has slight effect on O atom production. Under simulation conditions, the production and destruction of OH radicals is almost independent on the gas flow rate.

In addition, the main formation and destruction processes of O and OH, as well as the influence of dielectric constant of the substrate on the behaviours of O and OH have also been studied in this paper.

4. References

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