Kinetic chemistry modelling of atmospheric pressure plasma jets

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Atmospheric-pressure plasma jets (APPJs) have been gaining attention because of their great potential in various fields, e.g. surface treatment, environmental remediation and bio-plasma applications. In order to understand the underlying operating principles of such systems and to optimize their performance in applications, it is important to know the chemical kinetics of the reactive multi-species plasma. Recent results on modelling of gas-phase chemical kinetics in low-temperature atmospheric pressure plasma jets operated in an open-air environment are discussed.

1. Introduction

Atmospheric-pressure plasma jets (APPJs) have been gaining attention because of their great potential in fabrication of nano-materials or bio-plasma applications. In order to understand the underlying operating principles of such systems and to optimize their performance in applications, it is crucial to determine the evolution of the relevant species' densities and to reveal the underlying reaction chemistry, so that the composition of impacting species can be tailored to a specific application.

2. Modeling

A zero-dimensional time-dependent global plasma chemistry model with the extended reaction scheme to describe the complex plasma-induced non-equilibrium chemical network is introduced.

The complex plasma-induced chemistry of both the neutral and ionic compositions in atmospheric pressure He+0.5%O2 plasmas with humid air impurity is quantitatively revealed using the global model [1,2].

The present global plasma chemical kinetics model and simulation code describes a capacitively-coupled, rf-driven micro-scale APPJ (rf-μAPPJ) as the exemplar source [3]. This device was developed by Schulz-von der Gathen et al. [4, 5] on the basis of the original concept of Schütze et al. [6] but scaled-down and optimized for optical access. It consists of two plane-parallel stainless-steel electrodes enclosed by quartz windows along each side. One electrode is grounded, and the other is driven at a frequency of 13.56 MHz, using an rf power supply via an impedance matching network. This forms a core plasma channel of 30 mm length and 1 mm × 1 mm cross section. Considered throughout is a typical feed gas flux of 1 slm, which corresponds to a mean gas flow velocity of 17 m/s and a residence time in the core plasma region of about 2 ms. The gas pressure is 0.1 MPa (atmospheric pressure). The gas temperature in the core plasma region is set to 345 K.

Because of the presence of humid air, the plasma tends to produce significant amounts of reactive species and the plasma-induced chemical reactions are complex. So, here, the extended reaction scheme comprises over 1500 elementary reactions among 65 species.

Table I. Species considered

Neutrals	Carrier gas	He
	Admixture	O2
	Humid air	N2 (78.25%), O2 (20.97%), CO2 (0.03%), H2O (0.75%)
	Reactive species	He*, He2*, O, O(1D), O(1S), O2(1D), O2(1S), O3, O2v1, O2v2, O2v3, O2v4, N, N2v1, N2v2 N2v3, N2v4, N(2D), N(2P), NO, NO2, NO3, N2O
		H, OH, HO2, H2, H2O2, HNO, HNO2, HNO3
Ions	Positive	He+, He2+, O+, O2+, O4+, N+, N2+, N4+, NO+, H2O+, H3O+, H3O+.OH, H3O+.H2O, O2+ H2O
	Negative	O-, O2-, O3-, O4-, NO-, NO2-, NO3-, CO3-, CO4-, O2-.H2O, NO2-.H2O, NO3-.H2O, CO3-.H2O, CO4-.H2O
Electrons		Electrons

As discussed in [1,2], the explicit time-dependencies of the electron temperature and the production rate of metastable atomic helium (He∗, mostly in the lowest triplet state) in the centre of the plasma bulk, as well as the wall (electrode surface) loss rate of several key ionic species in the core plasma region, are at first obtained from one-dimensional (1D) simulations [3] for a He+0.5%O2 feed gas without other impurities and are then imposed in the global model. Our approach to employ input parameters from the 1D simulation yields information on the impact of the He∗ initiated plasma on the associated plasma chemistry. As for the core plasma region, the global model describes the chemical kinetics at the fixed source of the ionisation input, which would most closely correspond to a constant input power in the experiments.

3. Results

Figure 1 shows the temporal evolution of pronounced reactive neutral species in both (left-hand side) the core plasma region and (right-hand side) the effluent region of an rf-APPJ. The calculation is conducted with an air fraction air/(He +0.5%O2) = 0.025% (humidity of 50%). The O-atom density reaches a value of 5×1015 cm−3 at the exit of the core region then declines rapidly in the afterglow (Fig.1(a)). The maximum O2(1D) density at the jet' s nozzle is 7×1015 cm−3, which monotonically decreases in the afterglow. The O3 density, in contrast, gradually increases showing the trend to be saturated. The H and HO2 densities decrease in the afterglow (Fig.1(b)). While the OH density increases to reach a peak at around 0.5 ms, and then decreases after 3 ms. The densities of H2, H2O2, HNO2 and HNO3 increases in the afterglow. The N-atom density decreases dramatically (Fig.1(c)). The NO, NO2, NO3 densities stay nearly constant in the whole afterglow region. While, the N2O density increases by a factor of two after 3 ms.

4. Summary

In most applications helium-based plasma jets operate in an open-air environment. The presence of humid air in the plasma jet will influence the plasma chemistry and can lead to the production of a broader range of reactive species. The present global model can provide valuable insights into the underlying core and afterglow chemical reaction kinetics of atmospheric-pressure non-thermal plasmas.

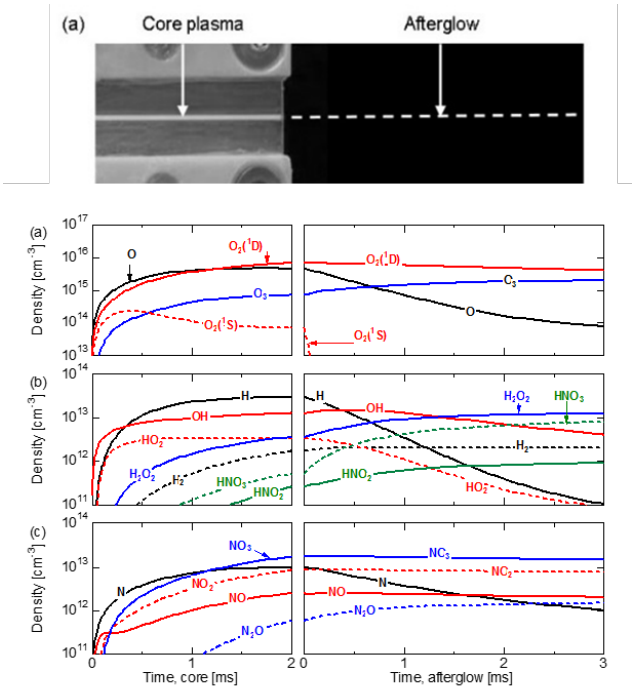

Fig.1. Core and afterglow species in an rf-driven He+O2+humid air plasma

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