Plasma chemistry in atmospheric-pressure He-O_2 plasmas in humid air

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We describe the influence of humid-air on reactive species in rf driven atmospheric-pressure helium-based plasmas in ambient air as determined through a zero-dimensional time-dependent global model. The effects of humid-air admixtures on the plasma-induced chemical reactions and the evolution of species concentrations in the helium-oxygen mixture (He-O_2, helium with 5000 ppm admixture of oxygen) are studied for wide air impurity levels of 0−500 ppm with the relative humidity of 0−100%.

For sensitive surface treatments in bio-medicine/bio-plasma applications, one of the most essential species is reactive oxygen species. Therefore, in the experiments using micro-scale atmospheric pressure plasma jets (μAPPJs), a small amount of oxygen is added to a carrier gas, helium. In order to further understand the underlying operating principles of the μAPPJ system and to optimize its performance in applications, it is important to know the chemical kinetics of a helium-oxygen (He-O_2) plasma containing a moist ambient air as an impurity. We describe the influence of humid-air on reactive species in the He-O_2 plasma for wide air fraction of 0-500 ppm with the relative humidity of 0-100% as determined through a zero-dimensional time-dependent global model. The code includes 700 reactions and tracks 59 species; neutral atoms and molecules, metastable species, vibrationally excited nitrogen and oxygen molecules, positively-charged ions, negatively-charged ions, various hydrate cluster ions and electrons.

Figure 1 shows the temporal evolution of the major (a) neutral biologically significant species and electrons, (b) positive ions and (c) negative ions concentrations during a 1 ms simulation at the air fraction of 500 ppm with relative humidity of 100%. Small windows in the figures [during 200 ms at final stage of 1 ms simulation] show that the densities of metastable helium atom (He*), O^+ and O^- are modulated with twice the driven frequency.

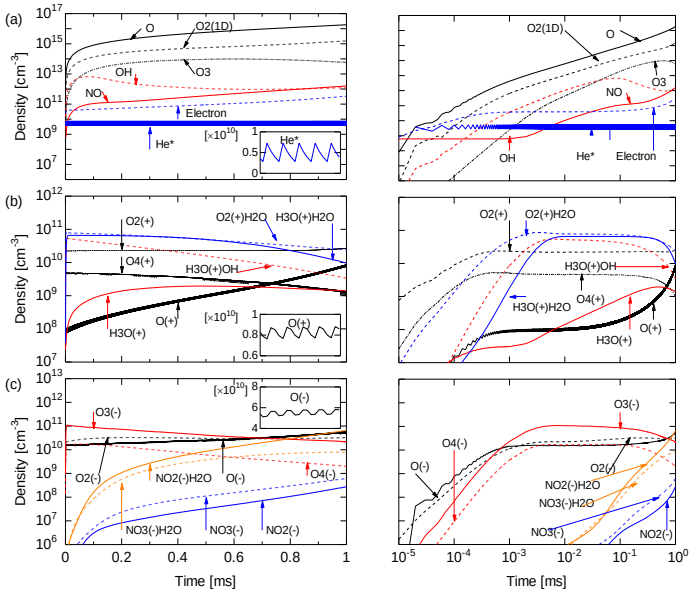

Fig. 1: Temporal evolution of (a) neutral species, (b) positive ions and (c) negative ions. Helium-based plasma with oxygen admixture (5000 ppm).The humid air impurity is 500 ppm (the relative humidity of 100%). Left-hand side: linear-time-scale plots. Right-hand side: log-time-scale plots.

A primary objective of the present work is to benchmark the predictions of the present global model against experimental measurements of some of the important plasma-produced species and also against the prediction of a 1D simulation which used a less extensive suite of species and reactions [1]. Figure 2 shows a bar chart of the absolute number densities of the 59 species included in the global model. The calculation is done for the number of air fractions ranging from 0 ppm to 500 ppm. In figure 2 the results for three operating conditions are considered in detail. In figure 2(a) the air fraction is 0 ppm and in figure 2(b) the air fraction is 500 ppm with relative humidities of 0% (black bars) and 100% (red bars). The open circles indicate the measured densities [1, 2]. The open triangles indicate the densities predicted by the 1D simulation with a reduced chemistry.

Comparing the global model and the 1D simulation it is perhaps not surprising that the densities calculated using the global model and by the 1D simulation are comparable across a wide variety of species. The more significant comparison is that between the global model and the experimental measurements. This suggests that the densities of reactive oxygen species, atomic oxygen (O), ozone (O_3) and siglet delta oxygen ($O_2(1D)$), and metastable helium atom (He*) calculated by the global model are reasonably consistent with those obtained from the experiments.

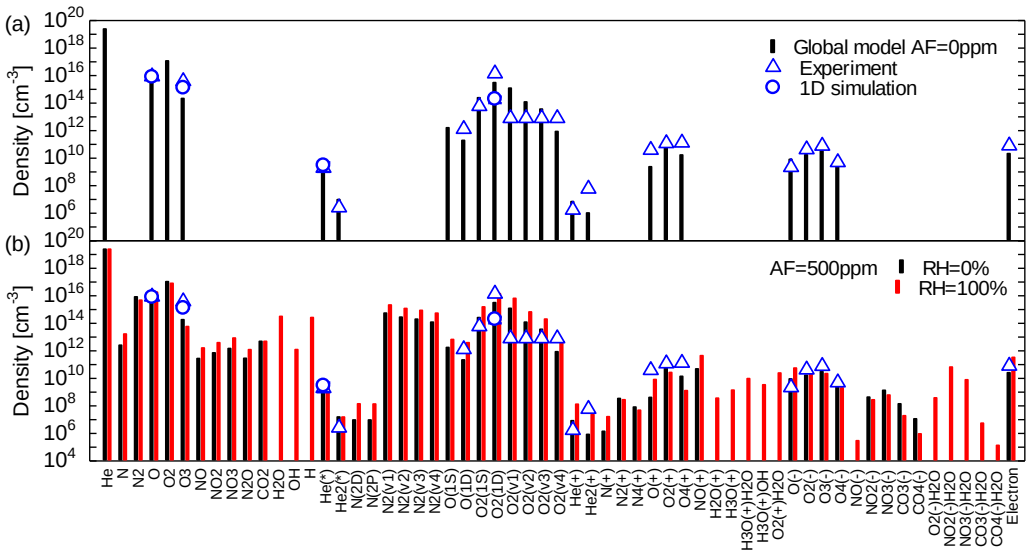

Fig. 2: A bar chart of the absolute number densities of the 59 species included in the calculated by the global model. (a) The air fraction is 0 ppm and (b) the air fraction is 500 ppm with relative humidities of 0% (black bars) and 100% (red bars).Open circles: measured densities. Open triangles: 1D simulation.

References

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