Water in low-temperature atmospheric-pressure plasmas

Felipe Iza

School of Electronic, Electrical and Systems Engineering, Loughborough University, Leicestershire LE113TU, UK

E-mail: f.iza@lboro.ac.uk

The non-equilibrium chemistry of water containing low-temperature atmospheric pressure plasmas has received growing attention in recent years for the potential use of these plasmas in biomedical applications, air treatment and chemical synthesis. As oxygen, H_2O is a good precursor of reactive oxygen species (ROS) and the two can be combined to create cocktails of ROS (O, OH, O_3, $^1O_2$, OOH and H_2O_2) of different compositions. These plasmas tend to be electronegative and display interesting dynamics, particularly when created in small gaps. From a practical point of view, it is important to understand the chemical pathways leading to the production of the biologically relevant ROS, as this will provide guidelines for the optimization of the plasma sources for a particular application.

We have analysed by means of 1-dimensional fluid simulations (60+ species, 850+ reactions), the key ROS and their generation and loss mechanisms in low-temperature water-containing atmospheric-pressure plasmas. Where possible, simulation results have been compared with experimental data and improved models with revised reaction rates and incorporation of rotational and vibrational excitation of water molecules have resulted in good agreement with experimental observations.

Although most ROS can be generated in plasmas with a wide range of oxygen and water admixtures, the chemical pathways leading to their generation change significantly as a function of the feed gas composition. The shift on the main chemical pathways governing the production of ROS implies that care must be taken when selecting reduced chemical sets to study these plasmas and has important implications in the reproducibility of plasma treatments performed in uncontrolled environments and/or samples.

The high reactivity of most of the ROS, however, limits their penetration into a treated sample and therefore encapsulation of the ROS and/or triggering of a secondary chemistry is required for the plasma treatment to reach beyond the first layers of biomolecules. Experimental and computational results suggest that production of ROS can be enhanced by the presence of water droplets, and combination of low-temperature plasmas with high speed droplets provide an interesting opportunity for the delivery of ROS beyond the surface of a treated sample.

This work was supported by the UK Engineering Physical Science Research Council.