Chemical pathways governing the production of Reactive Oxygen Species (ROS) in atmospheric pressure $He+O_2+H_2O$ plasmas

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It is well-known that atmospheric-pressure plasmas can be engineered to produce reactive oxygen species (ROS) and reactive nitrogen species (RNS) known to play important roles in biological systems. Here we concentrate on the generation of ROS, and in particular on the chemical pathways that govern the generation and loss of ROS in atmospheric pressure rf (13.56MHZ) plasmas sustained in helium with admixtures of O_2 and H_2O.

Both O_2 and H_2O are good precursors of ROS [1,2] and they can be combined to create cocktails of ROS of different compositions [3]. Due to the presence of O_2 and H_2O, these plasmas tend to be electronegative and display interesting dynamics, particularly when created in small gaps [4]. 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.

By means of 1-dimensional fluid simulations (61 species, 878 reactions), the key ROS and their generation and loss mechanisms are identified for admixtures containing 0-1% oxygen and 0-0.3% water content. Although most ROS can be generated in a wide range of oxygen and water concentrations, the chemical pathways leading to their generation change significantly as a function of the feed gas composition.

It is found that for a given oxygen concentration, the presence of water in the feed gas decreases the net production of oxygen-derived ROS (ozone, singlet oxygen and atomic oxygen), while for a given water concentration, the presence of oxygen enhances the net production of water-derived ROS (hydrogen peroxide, hydroxyl radicals and hydroperoxyl radicals). As a result oxygen rich mixtures tend to produce larger quantities of ROS whereas water rich mixtures produce cocktails with higher oxidation potential due to the presence of hydroxyl radicals.

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.

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References

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