Computational study on photochemistry in plasma-liquid systems

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One of the attractive features of atmospheric-pressure plasmas is its release of high-concentrated reactive oxygen and nitrogen species (RONS) into the ambient air or intended targets. As such plasmas have been utilized actively for biomedicine and more recently food and agriculture fields (aka plasma farming) particularly under a humid environment or direct contact with water, chemical characterization of plasma-liquid systems has become more important. In parallel to practical experiments, computational studies facilitate detailed insights into complicated chemical reactions. In this work, a special attention has been paid to photochemistry. We demonstrate that photochemical reactions induced by photons originated from plasma itself or external light sources are of profound importance and should be carefully considered in plasma-liquid systems. One example is the photolysis of RONS in the gaseous and aqueous phases; the distribution of both gaseous and aqueous species strongly depends on the photolysis of HONO, H_2O_2, and O_3. For this computational study, we have developed and used a numerical code which mainly solves continuity equations for zero-dimensional (0-D) plasma modeling and for 1-D gas and liquid modeling. The code provides the spatiotemporal evolution of each species from the discharge to the liquid region. Along with a brief description of computational modeling, detailed results associated with the gaseous and aqueous photochemistry will be presented.