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Liquid-phase chemically reactive species generated by water discharges or atmospheric-pressure discharges

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When water is exposed to atmospheric-pressure plasma (APP) generated in ambient air or discharges are generated in water, chemically reactive species such as reactive oxygen species (ROS) and reactive nitrogen species (RNS) are generated in water. The purpose of this research is to understand what kinds of chemically reactive species are generated and how they are transported in water exposed to such discharges. For this purpose, we have developed a numerical simulation code and also performed a variety of experiments, using low-frequency APP jets in ambient air and pulsed discharges in water. As to the numerical simulations, the governing equations are reaction-diffusion-advection equations coupled with Poisson equation. The rate constants, mobilities, and diffusion coefficients are obtained from the literature. The gaseous species are given as boundary conditions and time evolution of the concentrations of these chemical species in pure water is solved numerically as functions of the depth in one dimension. It has been found that, when a water surface is exposed to an APP, a variety of species are generated from the chemical reactions, especially in a thin liquid layer at the gas-liquid interface. Highly reactive species that are supplied to water from the APP are confined to this thin layer due to their high-rate reactions whereas less reactive and therefore more stable species such as H₂O₂ diffuse into water. This thin liquid layer, which may be called "reaction boundary layer," acts as the source of reactive species observed in the liquid bulk. The simulation results have also shown that ONOOH and O₃⁻, which are relatively stable and therefore easily transported by diffusion and advection to the depth, generate highly reactive OH radicals in the bulk water as if they transported OH radicals to deeper water. On the other hand, in the case of water discharges, a large amount of ozone is generated in water and diffuse into air and ozone seems to be the major oxidizing agent under such conditions.