Global simulation of chemical reactions in a NaCl solution exposed to an atmospheric-pressure plasma

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The interactions of atmospheric-pressure plasmas (APPs) with solutions containing Cl^- ions have been studied by many researchers. In such solutions, interactions of ROS and RNS with Cl^- can form various chlorine compounds. Some chlorine compounds, such as hypochlorous acid (HOCl) may be used as a disinfectant. The objective of this study is to understand how chlorinated water can generate chlorine-based disinfectants when it interacts with an atmospheric-pressure plasma (APP). Especially we aim to understand how such an exposure can suppress the generation of hydrogen peroxide (H_2O_2) in the solution, as shown in Ref. [1]. In this study, we performed global (i.e., zero-dimensional) numerical simulations of chemical reactions in NaCl solutions exposed to APPs. The reactive chemical species that enter the solution with their thermal velocities were taken as boundary conditions. In the global model, it is assumed that the solution is mixed rapidly, so that the concentrations of chemical species in the solution are assumed to be uniform. Our simulations showed that when a NaCl solution is exposed to oxygen-containing plasmas (e.g., an Ar plasma discharge with O_2 or H_2O), hypochlorite ClO^- is formed from the reaction between incident O atoms and Cl^- ions in the solution, which eliminates H_2O_2 in the solution through the reaction path $ClO^- + H_2O_2 \rightarrow Cl^- + H_2O + O_2$. Our simulation results agree qualitatively with the experimental observations of Ref. 1. Figure 1 shows that the decrease of the concentration of H_2O_2 (blue curve) as a function of the ratio of O and H_2O_2 concentrations in the gas phase.

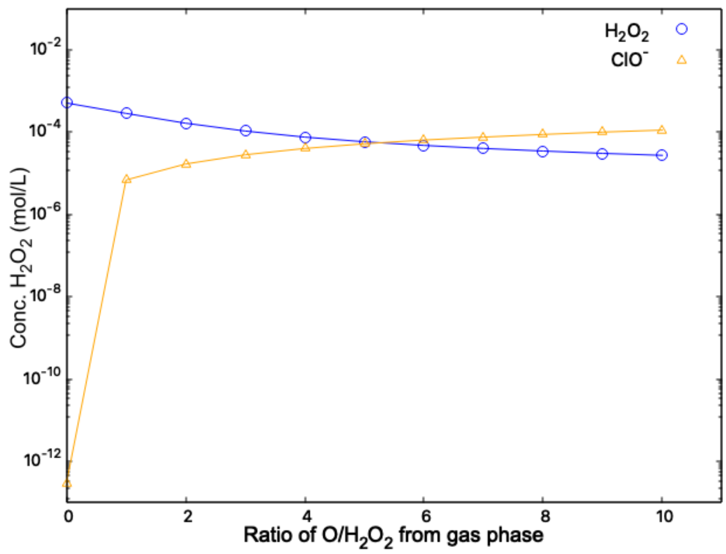

Figure 1. Concentrations of H_2O_2 and ClO^- in a NaCl solution as functions of the ratio of O and H_2O_2 concentrations in the gas phase.

[1] K. Wende, et al., "Identification of the biologically active liquid chemistry induced by a nonthermal atmospheric pressure plasma jet," Biointerphases10, 029518 (2015).