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Numerical simulation of the generation of reactive oxygen and nitrogen species (RONS) in water by atmospheric-pressure plasmas and their effects on Escherichia coli (E. coli)[1] KAZUMASA IKUSE, SATOSHI HAMAGUCHI, Osaka Univ — We have used two types of numerical simulations to examine biological effects of reactive oxygen and nitrogen species (RONS) generated in water by an atmospheric-pressure plasma (APP) that irradiates the water surface. One is numerical simulation for the generation and transport of RONS in water based on the reaction-diffusion-advection equations coupled with Poisson equation. The rate constants, mobilities, and diffusion coefficients used in the equations are obtained from the literature. The gaseous species are given as boundary conditions and time evolution of the concentrations of chemical species in pure water is solved numerically as functions of the depth in one dimension. Although it is not clear how living organisms respond to such exogenous RONS, we also use numerical simulation for metabolic reactions of Escherichia coli (E. coli) and examine possible effects of such RONS on an *in-silico* model organism. The computation model is based on the flux balance analysis (FBA), where the fluxes of the metabolites in a biological system are evaluated in steady state, i.e., under the assumption that the fluxes do not change in time. The fluxes are determined with liner programming to maximize the growth rate of the bacteria under the given conditions. Although FBA cannot be directly applied to dynamical responses of metabolic reactions, the simulation still gives insight into the biological reactions to exogenous chemical species generated by an APP.

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