Current Status and Future Challenges in Modeling and Numerical Simulation for Plasma Medicine

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In plasma medicine, plasmas are used directlyor indirectly to give stimuli to biological systems. For therapeutic purposessuch as wound healing and cancer therapy, plasmas may be applied directly toliving animal/human tissues. Since such tissues are typically covered with bodyfluids, reactive oxygen/nitrogen species (RONS) generated in the gas-phaseplasma may undergo reactions with molecules dissolved in the liquid, includingwater molecules. Plasmas are also used for the functionalization of biomaterialsurfaces, e.g., the improvement of surface hydrophilicity or the deposition ofspecific functional groups. The goal of this study is to understand how plasmagenerated species such as RONS interact with a liquid or (bio) materialssurfaces. For this purpose, we examine plasma-water interaction andplasma-solid interaction using numerical simulations. For plasma-waterinteraction, macroscopic reaction-diffusion-advection equations for allassociated species are solved for given fluxes of incident species from the gasphase. For the sake of simplicity, we only consider water as the solvent and assumethat the solution is dilute. The amount of electrolytes and their mobility determinethe resistivity of the solution, which then determines the current and chargedistributions in the liquid. For plasma-solid interaction, molecular dynamics(MD) simulations are used to analyze atomic-level surface modification. Themain concern here is the modification of chemical nature of the biomaterialsurface, including the formation or deposition of specific functional groups onthe (typically polymer) surface. In this presentation, our recent work in thesetopics is reviewed and a comparison of simulation results with experimental observationsis also discussed.