

Exploring the Interface Between Plasmas and Liquids: Addressing Contemporary Challenges with Innovative Software Tools

Tuesday, September 19, 2023 4:00 PM (30 minutes)

The interaction between low-temperature plasmas and liquid surfaces is a critical problem in many emerging plasma applications including plasma medicine, chemical processing, and water treatment, where precise control over the generation of reactive oxygen and nitrogen species, as well as solvated electrons, is essential. However, comprehensively characterizing the plasma-liquid interface poses significant experimental and computational challenges due to the complex multiscale and multi-physics nature of the problem. In this talk, we present an overview of recent advancements in modeling techniques for studying plasma-liquid interfaces, introducing (1) a novel open-source software package, Zapdos-CRANE, built upon the MOOSE finite-element framework; (2) RustBCA, a novel software for kinetic treatment of ion-surface interactions; and (3) hPIC2, a Particle-in-Cell for HPC simulations of multi-species chemically reacting plasmas. We demonstrate the code capabilities over several verification and validation problems. We then examine in detail a humid argon DC plasma over a water surface, operating in both cathodic and anodic modes. Within this system, we analyze the chemical pathways involving the formation and dissolution of hydroxide (OH) radicals, leading to subsequent hydrogen peroxide (H₂O₂) production. The model enables the investigation of key plasma-chemistry reaction mechanisms responsible for peroxide generation. Interestingly, our analysis reveals that anodic plasma treatment leads to an increase in hydrogen peroxide due to elevated water vapor dissociation reactions near the interface. Finally, we discuss the role of solvated electrons generated during cathodic plasma operations, demonstrating their direct degradation of hydrogen peroxide within the first nanolayers of the aqueous phase, consequently inhibiting its accumulation.

Speaker's Affiliation

University of Illinois at Urbana Champaign

Member State or IGO/NGO

United States

Primary author: CURRELI, Davide (University of Illinois at Urbana Champaign)

Presenter: CURRELI, Davide (University of Illinois at Urbana Champaign)

Session Classification: Water Treatment

Track Classification: Water Treatment