Controlling Plasma Reactivity Transfer to Gases, Solids and Liquids*

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Plasma discharges at atmospheric pressures allow efficient transfer of electrons' kinetic energy to chemical potential. In the process of breaking of bonds of molecular gases, plasmas produce high densities of reactive species. These species can then be utilized to treat flue gases and waste-water. However, currently-deployed systems suffer from poor energy efficiencies and throughputs, largely due to the lack of understanding of the underlying physics and chemistries. In this work, computational modeling efforts were put forth to elucidate the transfer of reactivity from plasmas to gases (via Packed Bed Reactors (PBRs)), solids (metallic catalysts) and liquid (micron-scale aerosols). The work was performed using the plasma hydrodynamics model – *nonPDPSIM* – developed and maintained in Prof. Mark Kushner's group. Necessary changes and updates to the code included addition of source terms to surface heating module, implementation a new mesh generator, and parallelization of radiation transport routines.

The evolution and properties of plasmas in the PBRs were characterized. Three plasma modalities were shown to exist, each leading to different rates of production of reactive species. Chemical selectivity could be achieved by choosing the packing fraction and materials which lead to preferential formation of one of the modalities over others. When metallic catalysts were added to the PBR, the discharge modalities changed, causing increased fluxes of charged species to the surfaces of the catalysts. This was, in part, due to realignment of charges within the metallic particles, which induced high local electric fields, and substantial numbers of field-emitted electrons. The high fluxes could lead to heating and self-cleaning of the catalysts, which would explain some of the plasma-catalytic synergy seen in literature. Lastly, the interactions of liquid aerosols with Dielectric Barrier Discharges were investigated. The diameter of the droplets was shown to address transport limits by maximizing the surface-to-volume ratio. Large surface area enabled rapid solvation from the gas-phase while small volume led to fast saturation of liquid-phase reactive species. Different species were shown to have different saturation time-scales, depending on the droplet size, pointing to an additional control mechanism of liquid-chemistry and selectivity.

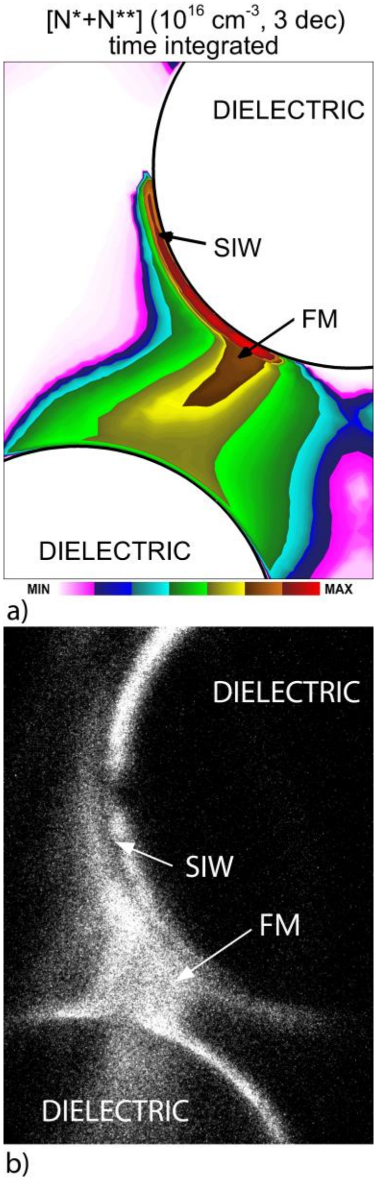

Figure 1. (a) Modeling results showing densities of light-emitting species between dielectric rods in a Packed Bed Reactor (b) Experimental ICCD imaging of a discharge in similar setting.

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