A Global Model for the Atmospheric Pressure Plasma Surface Functionalization of Polystyrene*

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Atmospheric plasma surface treatment is commonly used in industry to improve adhesion and wettability of bulk commodity polymers, such as polypropylene (PP), polyethylene, and polystyrene (PS) for uses in biomaterials and biomedical devices [1]. Treatment of polymers by plasmas involves the abstraction of H from the polymer backbone by O atoms or OH radicals to form alkyl radicals on the PS surface. O_2 can then be fixed to the alkyl sites to lower surface energy, resulting in increased wettability and adhesive properties. Correlating plasma operating conditions with fractional surface coverage of O-containing groups would help be valuable for process design of plasma functionalization systems.

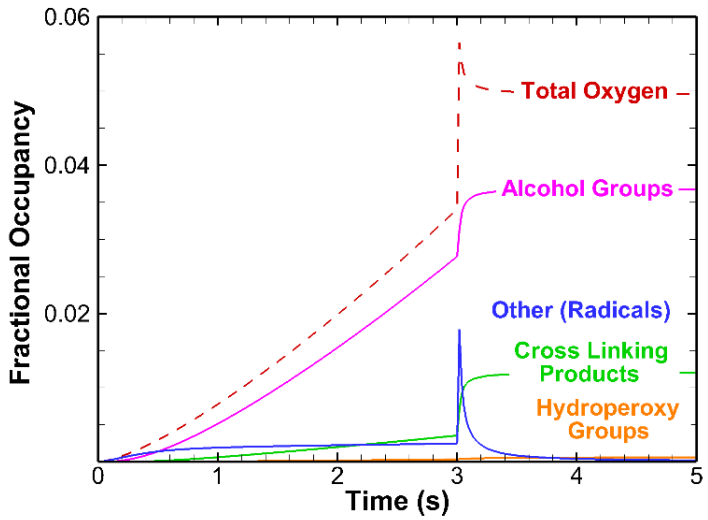

Figure 1 – Oxygen containing functional groups on PS surface after treatment by He/O_2 plasma jet and exposure to ambient air. (He/O_2 = 0.976/0.024, 270 W, Web Speed = 400 mm/min)

In this work we computationally investigate surface functionalization of PS using He/O_2 plasma jets. GlobalKin, a 0-dimensional global plasma chemistry model was used to simulate an RF driven plasma jet exiting into room air onto a PS surface situated a few mm from the reactor outlet. A surface site balance module [2] was used to predict fractional occupancy of oxygen on the PS surface after treatment due to gas phase-surface and surface-surface reactions. Results for trends in the fractional coverage by O-containing functional groups as functions of power, oxygen inlet fraction, web speed, relative humidity of room air, and PS distance from the nozzle after exposure to ambient air will be discussed. Results from the model will be validated by comparison to experimental trends for water contact angle measurements.

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References

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