ORAL PRESENTATION

Molecular Modeling of Polymer Composite Interactions with Analytes in Electronic Nose Sensors for Environmental Monitoring in International Space Station

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The ability to monitor the constituents of air in a closed environment is important to NASA for controlling the breathing air quality abroad a space shuttle/space station. The Electronic Nose (ENose) sensor developed at JPL for environmental monitoring in a crew habitat of a spacecraft uses arrays of polymer-carbon black composite sensing films. The selection of sensing films to achieve selectivity, sensitivity and stability for a particular task is difficult based on the traditional "trial-and-error" methods. Hence, an approach based on molecular modeling will not only help in providing fundamental understanding of the molecular level processes related to polymer composite-analyte interactions but also will set protocols for optimizing the array matrix.

The underlying objective of this work is to develop molecular models which accurately describe polymer-carbon black (CB) composite films used in the ENose sensors and to gain a detailed understanding of their interactions with analyte molecules that need to be detected for monitoring the breathing air quality in the International Space Station. The polymer model is based on its tacticity and connectivity while the carbon black is modeled as cluster of naphthalene rings (with no hydrogens). The molecular model of the composite film is obtained by adopting a strategy that involves inserting naphthalene rings in the voids of the polymer matrix followed by performing molecular dynamics (NPT-MD and NVT-MD) simulations first under "no solvent" and then under "solvent" conditions so as to mimic the experimental conditions. Dreiding 2.21 Force Field is used for the polymer and analyte molecules while the graphite parameters are assigned to the carbon black atoms. Polymers considered for this work include poly(4-vinylphenol), polyethylene oxide, methyl vinyl ether/maleic acid copolymer and Ethyl Cellulose. The target analytes are representative of both inorganic (CO2, NH3) and organic (methanol, toluene, hydrazine, Freon 113 etc.) classes of compounds. The composite model obtained will be used to study its microstructure as well as interactions with the analyte molecules. The composite-analyte binding interactions will be analyzed in detail for contributions from individual energy terms (van der Waals, electrostatic and H-bonding). Recommendations for selecting composite films for the ENose sensors will be made based on the validity of the molecular model determined by comparing its predictions to the experimental observations.

Key Words: Electronic Nose, Polymer composite, Molecular modeling, Interactions