Molecular Modeling of Interactions in Electronic Nose Sensors for Environmental Monitoring in Aerospace Applications

A. V. Shevade*, M. A. Ryan, M. L. Homer, A. M. Manfreda, S.-P. S. Yen, H. Zhou, and K. Manatt

Jet Propulsion Laboratory, California Institute of Technology
4800 Oak Grove Drive, Pasadena CA 91109

The ability to monitor the constituents of air in a closed environment is important to NASA for controlling the breathing air quality aboard the space shuttle and space station. The Electronic Nose (ENose) developed at JPL for environmental monitoring in a crew habitat uses arrays of polymer-carbon black composite sensing films.

Optimizing the array matrix for a particular task or group of analytes requires a fundamental understanding of the composite-analyte interactions. 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 molecular model of the composite film is obtained by adopting a strategy that involves 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 of film deposition. 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 o-vinyl pyridine, p-vinyl pyridine and epichlorohydrin. The target analytes are representative of both inorganic (CO2, NH3) and organic (methanol, isopropanol, acetone, toluene, indole) classes of compounds. The composite model obtained will be used to study the films microstructure as well as interactions with the analyte molecules. The validity of the model will be determined by comparing its predictions to experimental observations.

Selecting polymer sensing films to achieve selectivity, sensitivity and stability for a particular task is difficult based on the traditional "trial-and-error" methods. We also report a molecular modeling effort based on Monte Carlo simulations (MC) to guide experiments to select polymers for detecting dimethyl sulphide and hexane. The strategy involves calculating energy of mixing for the polymer-analyte interactions using the binding energies and coordination numbers of the components polymer and analyte. The theoretical predictions will be compared to the experimental data.

Key Words: Electronic Nose, Polymer composite, Aerospace application, environmental monitoring, Molecular modeling, Interactions