Evaluating Polymer/Polymer-Carbon Black Composite Coated Quartz Crystal Microbalance Sensor Response: An Experimental and Molecular Modeling investigation

B. Lin, A V. Shevade, M. A. Ryan, M. L. Homer, A. Kisor and A.M. Manfreda

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

Piezoelectric sensors such as the quartz crystal microbalance (QCM) have played an important role in probing interfacial processes at surfaces and thin films. Their high sensitivity and conceptual simplicity have resulted in wide range of applications as both chemical and biosensors in gas/liquid phases.

We report a combined experimental and molecular modeling effort to study how polymer-based sensors respond to organic vapors at the 24 hour Spacecraft Maximum Allowable Concentration (SMAC) ranges specified by NASA. The objective of this work is to determine the role of carbon black in the sorption process. This is achieved by calculating the partition coefficients for vapors in polymer and polymer-carbon composite films by measuring the mass uptake of an analyte by QCM sensors coated with those films. Systems under investigation include the detection of isopropanal at 100 - 600 ppm using Ethyl Cellulose and Ethyl Cellulose-Carbon composite (10 wt% carbon black) sensing films. Experiments are performed under dry (0% Relative humidity) and wet (45 and 60% RH) conditions.

The molecular modeling approach involves using Monte Carlo (MC) and Molecular Dynamics (MD) based techniques to evaluate the partition coefficients. Dreiding 2.21 Force Field is used for the polymer and analyte molecules, while the graphite parameters are assigned to the carbon atoms in the carbon black structure. Carbon black is modeled as clusters of naphthalene rings with no hydrogens in the polymer matrix. The effect of individual components in the polymer composite will be analyzed for its interactions with the analyte by calculating the energies of interaction for polymer-analyte, carbon black-analyte and polymer composite-analyte. The predicted partition coefficient values will be compared with those measured. These efforts are in parallel to the Electronic Nose (ENose) developed at JPL, which uses an array of conductometric polymer-carbon composite sensors that change resistance when exposed to vapors. This work complements the JPL ENose efforts by providing more understanding of the sensing phenomena and determining the candid polymer sets that may be used in the future.

Keywords: Piezoelectric, Sensor, Polymer-Carbon composite, Spacecraft Maximum Allowable Concentration, Partition coefficient, Molecular modeling