Detection of Organic Vapors by Polymer-composite coated Quartz Crystal Microbalance: An Experimental and Modeling study

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The extreme sensitivity and simplicity of a quartz crystal microbalance (QCM) has provided wide analytical possibilities for applications in environmental protection, biotechnology and medicine. QCM sensors are generally fabricated by coating the quartz crystal with functional thin films (organic/inorganic), which can interact with the analyte to be detected. In the present study, we investigate a QCM coated with polymer-carbon black composite to detect organic vapors at the 24 hour Spacecraft Maximum Allowable Concentration (SMAC) ranges specified by NASA. These experiments 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. The polymers used for the composite films are ethyl cellulose and polyethylene oxide. The carbon black (Cabot Black Pearls 2000) is used as the filler. The organic analytes tested are water, isopropanol and toluene. The experimental results were analyzed by calculating the mass up take and partition coefficients. A molecular modeling approach using grand canonical Monte Carlo simulations (GCMC) was also used to predict both mass up take and 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 was analyzed for its interactions with the analyte by calculating the polymer-analyte, carbon black-analyte and polymer composite-analyte interactions. The predicted partition coefficient values are then compared with the one measured by experiments.

Keywords: QCM, sensor, Polymer composite, Organic vapor, Spacecraft Maximum Allowable Concentration, Molecular modeling