Environmental Monitoring by Electronic Nose Sensors: A Molecular Modeling Study

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The Electronic Nose (ENose) has been developed at JPL for environmental monitoring in the crew habitat of a spacecraft. The sensing array is made up of polymer-carbon black (CB) composite sensing films. Optimizing the array matrix for a particular task or group of analytes requires a fundamental understanding of the composite-analyte interactions. We report a molecular modeling effort initiated to develop understanding of the interactions of polymer-CB composite films with analytes. The composite model involves clusters of naphthalene rings (with no hydrogens) representing the CB incorporated in the polymer matrix, which is modeled by its tacticity and connectivity. Dreiding 2.21 Force Field is used for the polymer and analyte molecules while graphite parameters are assigned to the carbon black atoms. Molecular dynamics technique is used to obtain the equilibrium composite structure. The polymers investigated for this work are poly(4-vinylphenol) and polyethylene oxide. The solvent analytes include the compounds 2-propanol, acetone and toluene, representative of alcohol, ketone and aromatic compounds, respectively. The composite model obtained is studied for its microstructure as well as its interactions with the solvent molecules. The validity of the model will be determined by comparing its predictions to experimental observations.

Keywords: Electronic Nose, Environmental monitoring, Polymer composite, Molecular modeling