Correlating Electronic Nose sensor response for air quality monitoring: An Experimental and Modeling Study

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The Electronic Nose (ENose) sensor developed at JPL uses arrays of polymer-carbon black (CB) composite sensing films for environmental monitoring in crew habitat of spacecraft. Each sensor is non-specific to any one vapor. Upon exposure to a vapor, the sensors respond, creating a pattern across the array. Modeling and correlating experimental sensor response or activity with a descriptor set or independent variables using multivariate statistical techniques such as Quantitative Structure-Activity Relationships (QSAR) will provide a better understanding and insight into the possible factors affecting the sensor response. The descriptor set consists of parameters that describe sensor material (e.g., cohesive energy, dipole of the polymer) and sensing phenomena (sensing film-analyte interaction energies). These are calculated using inputs from molecular modeling tools and other empirical and semi-empirical predictive methods such as Quantitative Structure–Property Relationships (QSPR).

In the current investigation we report a combined experimental and modeling effort to study the sensing of organic vapors at the 24 hour Spacecraft Maximum Allowable Concentration (SMAC) ranges specified by NASA using polymer- carbon black composite films. A set of 16 polymers are used for sensing a homologous series of alcohol (methanol-butanol). The polymers used in the composite film are categorized in four categories, (i) Hydrogen bond basic (ii) Dipolar and hydrogen bond basic Moderate dipolarity (iii) weak hydrogen bonding and weakly dipolar (iv) weak or no hydrogen-bonding. The polymer descriptors calculated using QSPR technique range from structural, spatial, topological, conformational, and thermodynamic properties of the polymer. The sensing phenomena is described by the polymer-analyte interaction energies and are calculated using molecular modeling and simulation tools. QSAR studies using Genetic Function Approximations (GFA) were performed to achieve the best correlation between each sensing film and the alcohol homologous series. Prediction of a sensor activity for a different alcohol (whose experimental activity is known and was not used in formulating the correlation) was tested to determine the validity of the correlation.

A validated correlation for the sensor activity could be used *a priori* to predict responses of potential sensors to new analytes in a given homologous series or family class (alcohol, aromatics etc.). Thus, experimental efforts coupled with theoretical and computational approaches will be a key in less extensive experimental testing and will provide guidelines to select sensor materials in a more rational way.

Key Words: Environmental monitoring, Electronic Nose, Polymer composite, QSAR, Molecular modeling,