A Quantitative Structure-Activity Relationship (QSAR) study to describe Electronic Nose Sensor Response

A. V. Shevade, M. A. Ryan, A. M. Manfreda, H. Zhou,
M. L. Homer, B. Lin, A.K. Kisor.
and K. Manatt

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

A rational way to design and select materials for engineering applications could be achieved by coupling experimental and theoretical efforts. We are interested in evaluating the performance of materials used as sensing media in sensor devices. 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 and creates a pattern upon exposure to a vapor. Correlating the sensor experimental response with molecular descriptors will provide an insight on the molecular parameters affecting the device performance. One such method to achieve this is the Quantitative Structure-Activity Relationships (QSAR), which is a multivariate statistical technique that correlates activity with a descriptor set (independent variables). The activity is the sensor response. The descriptor set consists of parameters that describe intrinsic properties of both the sensor material and target molecules (analytes) as well as sensing film-analyte interaction energies that decide the sensing phenomena.

In the current investigation, we report a combined experimental and modeling effort for the JPL ENose to study the sensing of organic vapors at the 24-hour Spacecraft Maximum Allowable Concentration (SMAC) ranges specified by NASA. The experimental data was obtained for 18 target analytes using a set of 4 chemically different polymers (e.g., Hydrogen bond basic, weak hydrogen bonding and weakly dipolar etc.). The descriptors for the polymer and analyte are calculated using Quantitative Structure-Property Relationships (QSPR) techniques and consist of structural, spatial, topological, conformational, and thermodynamic properties. The polymer-analyte interaction energies are calculated using **molecular modeling and simulation tools**. QSAR studies using Genetic Function Approximations (GFA) are performed to achieve the best correlation between each sensor response and the molecular descriptors. For a given polymer, the experimental sensor response was correlated for the entire analyte set as well as analyte subgroup with similar chemical functionalities.

This talk will focus on the selection of descriptors for QSAR studies. We will discuss in detail the energy term calculations that describe the interactions between an analyte with components of the polymer-carbon composite system (polymer and carbon). The binding energy terms calculated include: polymer-analyte, and carbon black-analyte, polymer-carbon, polymer-polymer, and carbon black-carbon black pair interactions. The binding energy term calculated for each pair has contributions from van der Waals, electrostatic and hydrogen bonding energy terms. The binding energies are calculated using Monte Carlo technique and are averaged over 100000 pair configurations. This talk will also consider the descriptors which are intrinsic to the polymer sensor and to each analyte, such as glass transition temperature, molar refractivity, melting/boiling point, or density, and will discuss how it was decided for this study whether to include such descriptors in the QSAR correlations.

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