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An Atomistic Model of Polymer-carbon Composite Behavior to Predict Sensor Response

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The availability of a miniature, portable instrument capable of identifying contaminants in the breathing environment at parts-per-billion levels would greatly enhance the capability for monitoring the quality of recycled air as well as providing notification of the presence of potentially dangerous substances from spills and leaks. Such scenario exists on space shuttles/space station. To fill this need, JPL is developing an Electronic Nose (ENose) for air quality monitoring. The JPL ENose uses an array of polymer-carbon black composite sensing films. Our objective in the modeling portion of this work is to develop models that correlate with sensor response to a high degree of significance and reliability. Such models will provide a method to predict analyte responses for polymers where experimental data are not available. The ability to predict analyte responses is useful in selecting an array of polymer-based sensors to give distinct responses to a variety of analytes. It may also be extended to making identification of compounds for which patterns of response have not yet been recorded and stored in the sensor analysis library.

We report a study to correlate the ENose sensor data using molecular descriptors extracted from a polymer-carbon composite model. The experimental ENose data to be correlated are derived from polyethylene oxide (PEO) polymer-carbon composite sensing film responses to 18 target gas compounds at parts per million (ppm) concentration levels (**Table 1**). The model for the polymer-carbon composite is developed by inserting naphthalene rings (carbon black) in a polymer matrix, followed by using a combination of molecular mechanics (MM) and molecular dynamics (NPT-MD and NVT-MD) techniques for equilibration. The sensor activity is correlated by descriptors that define both the intrinsic analyte properties and molecular level descriptors for sensor response. The analyte descriptors are further classified into: Electronic, Spatial, Structural, Thermodynamic and Topological categories. The descriptors for sensor response are described by the molecular level interactions of the analyte in the polymer-carbon sensing film. The predicted sensor response model is formulated by using multivariate statistical methods: Quantitative Structure-Activity Relationship (QSAR).

The success of QSAR as a method to develop algorithms to predict sensor response depends greatly on the descriptors selected. As shown in **Figure 1**, QSAR has resulted in an algorithm which predicts concentration dependence response of PEO to selected analytes. This paper will discuss the selection of descriptors and the methods used to calculate molecular level descriptors.

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

Table 1 : List of analytes

1. Acetaldehyde
2. Acetone
3. Ammonia
4. Chlorobenzene
5. Dichloromethane
6. Ethanol
7. Isopropanol
8. Xylenes
9. Tetrahydrofuran
10. Trichloroethane
11. Acetonitrile
12. Ethylbenzene
13. Freon113
14. Hexane
15. Methyl ethyl ketone (MI
16. Methane
17. Methanol
18. Toluene

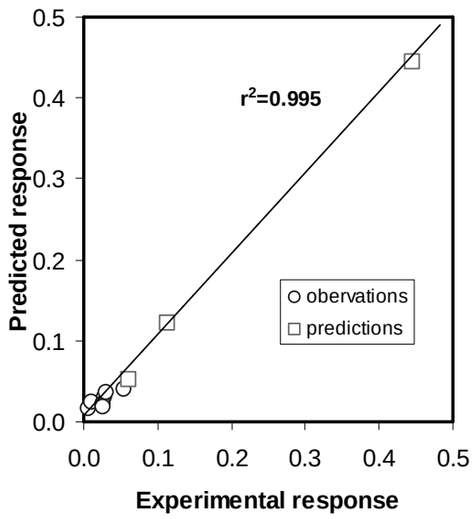

Figure 1: Predicted versus experimental sensor response for hydrocarbons excluding aromatics and including those containing oxygen are used as observations to form the model. The activities of aromatics: toluene, o-xylene and ethyl benzene are predicted. The model developed is found to be a function of polymer-analyte, analyte-water and analyte-analyte interactions. The sensor response = $A_1x + A_2x^2$, where x is the concentration. In the investigation we have used coefficients A_1 as activities for our QSAR studies.