1.6 Surface Acoustic Wave Array Detectors

Technology Need

Characterization, monitoring, and cleanup of contaminated DOE sites will require field deployable analytical techniques such as chemical sensors. Chlorinated hydrocarbons contaminate soil and groundwater at over ten DOE sites. At each individual site, concentrations found vary widely. Sensors used at these sites must be sensitive and selective, operate over a wide dynamic range, and suitable for deployment in field environments.

Technology Description

The purpose of this task is to design, develop, and demonstrate array sensor systems for sensing volatile organic compounds (VOCs), including chlorinated hydrocarbons and other vapors of interest, to environmental cleanup and occupational safety. These sensor arrays are based on polymer-coated SAW vapor sensors and data processing, using pattern recognition and chemometric techniques. Key elements of this effort include the rational choice of polymer materials for use as the selective sensing layers; a predictive method for sensor performance; experimental evaluation of sensor arrays for VOC detection; and pattern recognition and other chemometric techniques for converting data into chemical information.

The advantages of the SAW vapor sensor technology include the rugged planar design of the devices; the suitability of polymer-coated devices for use in arrays with pattern recognition; fast response times (seconds); rapidly reversible responses (the selective material is not altered by the vapor); high vapor sensitivities (ppm to ppb detection limits depending on the particular vapor); and the flexibility of the array approach to be adapted to many detection problems. The analyte(s) to be detected by a SAW sensor array system can be changed merely by the selection of the polymer coatings and the pattern recognition algorithm used.

The sensor array approach provides greatly increased selectivity and reliability in field environments over a single sensor. Single sensors cannot determine if an interfering species is present that might invalidate the measurement. In addition, sensor arrays offer the possibility of detecting and quantifying multiple analytes with the same system. The compact SAW sensor array systems envisioned will convert data into chemical information and communicate it in a form necessary for decision making. Thus, SAW sensor technology will become the basis for practical, fieldable solutions to characterization and monitoring problems.

This task is part of a collaborative effort in the development of SAW array systems. The team includes two National Laboratories and a number of commercial partners (see below). The task at PNNL is focused specifically on the scientific and technical aspects of selecting and using polymers as the sorbent layers on SAW sensors for sensor arrays.

Benefits

Appropriate sensing of VOCs during environmental cleanup will improve worker safety; aid in decision making on types of protective equipment required and length of time workers can stay in the environment; and reduce costs by measuring multiple vapors with a single instrument rather than requiring separate sensors for each vapor.

Collaboration/Technology Transfer

This work is being coordinated with SAW sensor development tasks at SNL. We have a funded collaboration with Sawtek, Inc, and General Atomics for the development and commercialization of SAW sensor array instruments.

Accomplishments

This task began with a modeling effort to develop a rational approach for the selection of polymeric sensor coating materials for SAW sensor arrays. This approach was based on using linear solvation energy relationships (LSERs) to model the sorption of vapors by polymers and predict polymer/gas partition coefficients. Using models for SAW sensor transduction mechanisms, these partition coefficients were converted to sensor responses. These models were validated against experimental sensor response data. Polymers offering optimal sensitivity for various classes of vapors were identified. Predicted limits of detection were compared with permissible exposure limits and threshold limit values. It was found that SAW vapor sensors could detect the majority of vapors considered at regulatory levels.

In addition, the modeling effort was used to compare the performance and selectivity of polymer materials with other novel materials appearing in the literature. It was found that assembled fullerene materials did not offer substantially different selectivities than low polarity polymers. Similarly, it was found that cavitand-type materials purported to operate via molecular recognition did not offer different selectivity than amorphous polymers. These results indicated that our original plan to use polymers as the selective layers on our sensors was appropriate.

Polymers for SAW vapor sensors have been screened in a large experimental program testing 20 different polymer materials as sensing layers against 19 vapors, each at four concentrations. Polymer-coated sensors were examined for film morphology, speed and reversibility of sensor responses, sensitivities to vapors, and linearity of calibration curves. In addition, chemometric techniques have been used to examine relationships among the test polymers.

Chemometric methods have also been used to examine the ability of arrays of polymer-coated sensors to discriminate and classify vapors. Dendrograms showed excellent clustering of vapor data as shown in Figure 1.6-1. Chemometric models were able to classify low polarity vapors by compound class; for example, aliphatic hydrocarbons, aromatic hydrocarbons, and chlorinated hydrocarbons. In further analysis, it was found that all the chlorinated hydrocarbon vapors tested (perchloroethylene, trichloroethylene, carbon tetrachloride, and dichloromethane) could be distinguished from one another as well as from all the other vapors.

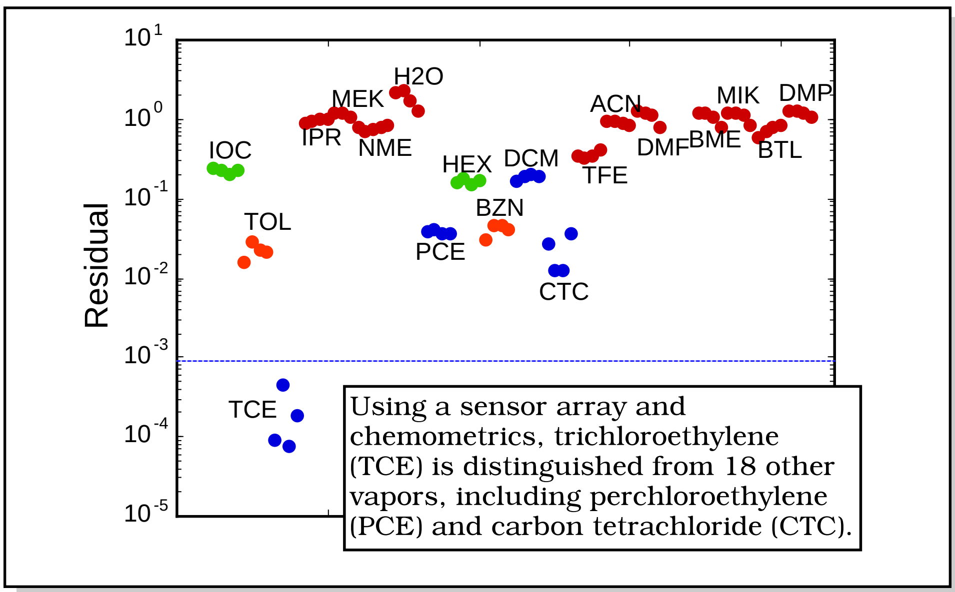

Figure 1.6-1 Results for the classification of trichloroethylene (TCE).

TTP Information

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BIBLIOGRAPHY OF KEY PUBLICATIONS

None available at this time.