Producing and Processing Microsensor Signals to Meet Critical Chemical Monitoring Needs

NIST scientists have developed a microsensor for detection in varied gas phase mixtures, of relatively low concentrations of a number of different toxic industrial chemical (TIC) analytes. The microsensors are based upon temperature programmed sensing technology using various transducing materials for very precise and sensitive chemical detection. Important progress has been made toward making tunable, widely deployable microsensors for utility in differing gas mixtures. Such sensors have application in environmental health and safety monitoring and in chemical threat detection for homeland security.

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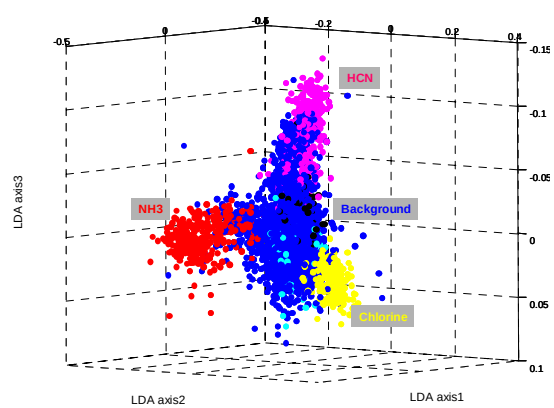
The United States currently faces a variety of terrorist threats, and it is increasingly affected by global warming. There are clear needs for efficient alternate energy sources, and demands better and more affordable health care for its aging population. These realities have created an unprecedented need for chemical sensing and monitoring technology that can positively impact the current human condition. These "front-end" chemical analysis needs are being realized at a time when computing and communication advances have produced a highly capable infrastructure for collecting, transferring and utilizing analytical data. Development of low cost chemical monitoring devices for diverse targets in substantially different applications, however, greatly lags behind the computing and communication support tools now available. In addition, due to cost and other logistical factors, existing analytical instruments can be deployed only in an extremely small fraction of the desired settings. In many cases, the analytical demand would best be met with robust, low-power, network-deployable/addressable microsensors.

Development of low cost chemical monitoring devices for diverse toxic industrial chemical (TIC) targets, will enable new innovations in homeland security, environmental and medical business sectors.

The detection of relatively low concentrations of a substantial number of different analytes in varied gas phase mixtures represents a broad and challenging problem for sensor researchers. Success in this endeavor, however, could provide critical measurement tools for diverse applications, and important progress has been made toward making tunable, widely deployable microsensors for utility in differing gas mixtures.

The NIST array technology combines ≈100-µm microhotplate elements with CMOS compatibility, nanostructured sensing films, and artificial neural network (ANN)/statistical signal processing to realize tiny monitoring devices that consume very little power and have been shown to be sensitive at the nmol/mol (ppb) regime and below. In order to recognize target species in variable backgrounds, the signal streams from our conductometric (chemiresistive) microsensors are enriched in two ways – multiple elements with differing sensing films are included in an array format, and each element is individually programmed to cycle through many temperatures as a function of time. The temperature programmed sensing (TPS) operation probes temperature-dependent interactions between the gaseous ambient and sensing materials within the array to produce analytically rich databases that can be analysed to recognize and monitor target molecules. The ultimate capability of these microsensor arrays depends on the selection of sets of transducing materials, the quality and stability of their responses, and the power of the response recognition software.

***Figure One:* Linear Discriminant Analysis of a four-element array response to different toxic industrial chemicals**



During the past year, we have made significant advances in developing statistical correlation measures to assess the orthogonality/similarity of responses from sensor materials; this ability greatly assists our selection of film

thicknesses and film compositions to incorporate within an array for specific detection application sectors. We have also employed dimensionality reduction techniques, such as linear discriminant analysis (LDA) and principal component analysis (PCA), for visualizing the sensor array response to determine whether sufficient analytical information is available using the chosen materials for species recognition. ***Figure 1*** shows a LDA plot of a 4-element sensor array response to three different toxic industrial chemicals (TICs). It can be clearly seen that the array response to ammonia, hydrogen cyanide and chlorine form clusters that are easily distinguishable from each other and the background. We have also been able to quantify the variation of signal baselines over extended operating times for our microsensors, and develop data preprocessing routines for drift compensation.

Figure 2 demonstrates the effect of our compensation approach, which allows previously trained recognition software to remain viable over months for detection of certain low level toxic industrial chemicals, even as a number of interfering compounds are introduced into the sampled background. These advances are critical to the production of pre-programmed microsensors that can operate in the field for near-real time with multi-species recognition relevant to homeland security, global warming, process control, and other applications.

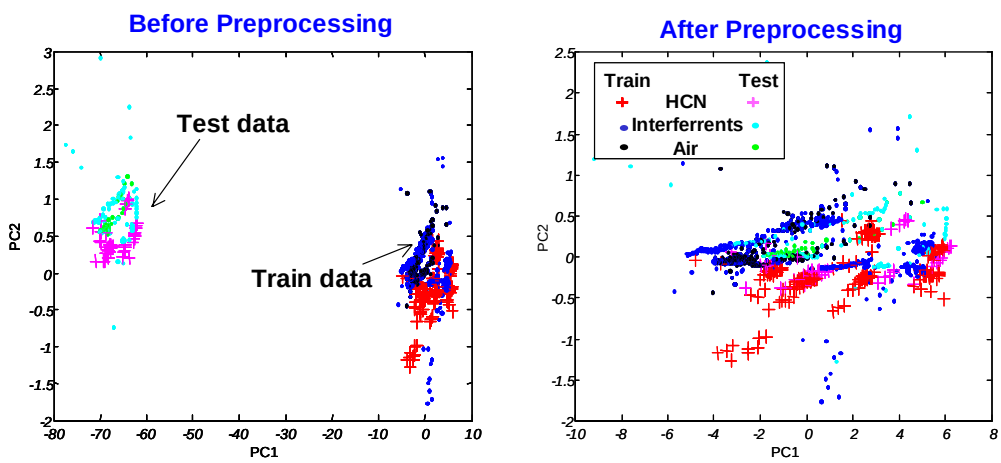


Figure 2*: *Illustration of the baseline correction technique (note the PC 1 axis scale change) necessary to allow pre-trained recognition software to remain viable for up to two months for detection of TICs.