

Detection of organic chemicals by SAW sensor array

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Accepted 22 March 1999

Abstract

A portable SAW sensor array instrument with integrated chemometric software has been developed to identify a variety of chemical classes like paraffinics, aromatics, chlorinated hydrocarbons, ketones and alcohols. The system was trained with known chemicals and a chemometric model was developed for two applications: bulk VOC identification and environmental monitoring of trace level VOCs. The instrument was then successfully tested in the lab and in the field for these two applications. The ability to identify and quantify these VOCs over a dynamic range from low ppm trace levels to high concentrations (close to the chemical's vapor pressure) was demonstrated. © 1999 Elsevier Science S.A. All rights reserved.

Keywords: Organic chemicals; SAW sensor array; Chlorinated hydrocarbons

1. Introduction

There is currently a need for low-cost portable instrumentation to identify and quantify volatile organic chemicals (VOCs). Manufacturers and end users of VOCs must correctly identify shipments in order to prevent dangerous and costly cross-contamination. In addition, trace levels of some VOCs in the air and water must be monitored to meet environmental regulations. Analytical techniques such as GC, MS or FTIR that are often used in these applications involve large, expensive instrumentation that has slow response time and does not lend itself easily to portability. Previous work has shown that instrumentation based on a SAW sensor array is a promising technique in this area due to the compact size and minimal power requirements of the SAW sensors [1–3].

2. System description

The instrument consists of an array of six SAW sensors coated with chemically selective polymer films, an inte-

grated sampling system, microprocessor and supporting electronics. It is a portable, self contained unit that is battery operated and will run for approximately 6–8 h under typical operating conditions before the batteries need to be recharged. The system was trained with known chemicals and possible interferants for two applications: bulk VOC identification and environmental monitoring of trace level VOCs. A chemometric model was developed for each application based on the training data. When exposed to an unknown chemical, the sensor responses are compared to the stored patterns and the chemometric model identifies and quantifies the sample, or indicates that it is an unknown chemical that was not part of the training data.

The system can operate in two modes: real time or preconcentrated. The real time mode is applied for medium to high chemical concentrations close to the chemical's vapor pressure and has a response time of less than a minute. The preconcentrated mode is used for low chemical concentrations less than 50 ppm. The complete operating cycle (load, desorb and sensor response) is between 5 and 20 minutes depending on the application.

3. Results and discussion

For the bulk chemical ID application, a head space gas sample of each industrial solvent was taken at three differ-

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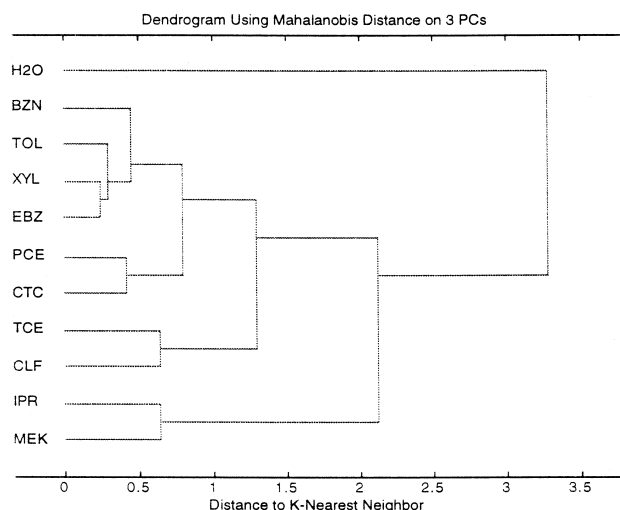


Fig. 1. K-NN cluster analysis of 10 VOCs and water.

ent concentrations and injected into the system. The system correctly identified the samples and provided a confidence level with a response time of approximately one minute.

For the environmental monitoring application, the head space of ground water wells was sampled. The instrument demonstrated the ability to qualify and quantify single, or binary mixture of, VOCs over a broad dynamic range. A K-NN cluster analysis plot of 10 VOCs and water is shown in Fig. 1. Ten VOCs are benzene, ethyl benzene, toluene, *p*-xylene, trichloroethylene, perchloroethylene, carbon tetrachloride, chloroform, 2-propanol, methyl ethyl

Table 1

SAW sensor and GC measurement from an in situ bioremediation site

Sample date	Sample site	SAW sensor (TCE/PCE)	GC (TCE/PCE)
6/8/98	782-4M inlet	23/181 (ppm)	24/162 (ppm) ^{a,b}
6/8/98	782-4M stack	3/145 (ppm)	4/123 (ppm)
6/17/98	782-4M inlet	44/290 (ppm)	33/272 (ppm) ^a
6/17/98	782-4M stack	5/175 (ppm)	5/156 (ppm)

^aGC detected 5 ppm TCA.

^bGC detected 10 ppm chloroform.

ketone. Similar chemicals group together but each chemical is still separated. Linear relationship between sensor responses and chemical concentrations was observed for trichloroethylene using both the preconcentrated and real time modes as shown in Fig. 2. Table 1 compares the analytical results of TCE/PCE binary mixture as measured with the SAW sensor and GC at a DOE in situ bioremediation site. Most of the samples are in good agreement with the exception of those where concentrations of other gases, not included in the training data for the SAW sensor, were present.

4. Conclusions

A portable instrument based on a polymer coated SAW sensor array is an accurate reliable method for identification and quantification of VOCs. This instrument can be applied to both bulk chemical identification applications and environmental monitoring of trace level VOCs.

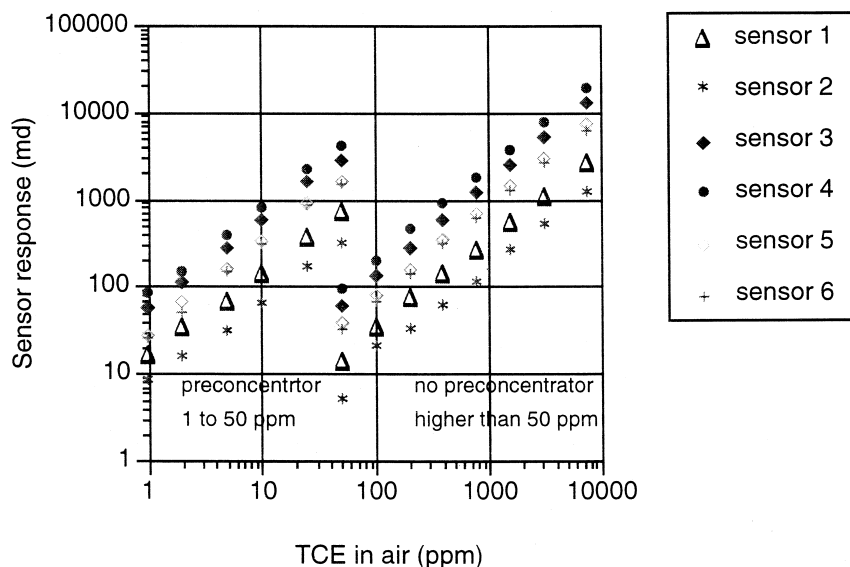


Fig. 2. Linear sensor responses to trichloroethylene from 1 to 10,000 ppm.

Acknowledgements

The authors thank Jay Grate of Pacific Northwest National Lab for his advise on sensor coating selection and support with sensor coating material. This paper was prepared with the support of the U.S. Department of Energy (DOE) Award No. DE-FC07-95ID13343. However, any opinions, findings, conclusions, or recommendations expressed herein are those of the authors and do not necessarily reflect the views of DOE.

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