ARRAYS OF SENSORS AND MICROSENSORS FOR FIELD SCREENING OF UNKNOWN CHEMICAL WASTES

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Abstract

The high cost of laboratory-based analysis has driven the development of rapid screening methods for hazardous chemicals in unknown wastes. Screening methods permit the "triage" of samples into those that (a) contain no regulated wastes, (b) definitely contain regulated chemicals, or (c) are ambiguous. Only the last category requires detailed analysis.

The requirements of portability and ease of use place extraordinary demands on the designers of analytical instruments. In this paper, we will discuss several approaches to obtaining qualitative analytical data from multiple sensors or highly-selective sensors. These are: (a) a sensor with a selectivity 1000-10000 times greater for chlorinated or brominated compounds than for unsubstituted ones; and (b) pyrolysis-EC, which uses catalytic pyrolysis, arrays of electrochemical sensors, and pattern recognition methods to identify pure chemicals and mixtures. Two applications of the latter are described, the rapid identification of chemical vapors, and the grading of grain according to "odor".

Introduction

The high cost of laboratory-based analysis has driven the development of rapid screening methods for hazardous chemicals in unknown wastes. A screening method is one that can be done on-site, by non-chemists, inexpensively and safely. On the other hand, a screening method is less likely to provide the definitive data that a full laboratory analysis, perhaps requiring GC/MS or ICP, might give. In the case where no information is available, however, even limited information can be of value, especially if it is used to supplement data gathered from other sources. For example, a suite of simple screening methods may be used for the "triage" of unknown samples into positive, negative, and ambiguous groups. Often, the nature of the chlorinated compounds may be known from purchase or production records, so that only the ambiguous category may require detailed analysis. Screening methods may also be useful for confirming conclusions that have already been drawn from independent data, for example, that a collection of similar barrels do indeed contain the same materials.

The willingness to accept reduced certainty for the sake of economy and practicality opens the door to a wide variety of useful techniques that can be used in the field. In this paper, we will describe two such methods.

A unique semiconductor sensor has been found that is very sensitive to chlorinated and brominated organic compounds (1-3). It shows no detectable response to hydrocarbons, oxygen- or nitrogen-containing organic compounds, or fluorocarbons.

A second method that has given us promising results has been catalytic pyrolysis of chemical vapors combined with electrochemical detection. Compounds that are not normally thought of as electrochemical analytes, such as chloroform or cyclohexane, can be partially oxidized on a hot platinum surface (4). The volatile products always include some that give a response on a porous-electrode electrochemical sensor. We have confirmed over several years that the products of the pyrolysis are reproducible for most organic and some inorganic compounds when the conditions are kept reasonably constant (5). We have also confirmed the critical requirement that the products are independent of analyte concentration, at least at concentrations of below 200 ppm. We call this method **pyrolysis-EC**.

The present embodiment of pyrolysis-EC is an instrument we call the CPS-100. This device uses an array of electrochemical gas sensors with different, but overlapping, selectivities. The incoming gases are pyrolyzed over noble metal catalysts heated at controlled temperatures. The operation of the instrument is orchestrated by a fairly powerful computer which can perform pattern analysis on the resulting data. In this paper, we report the results of a study on pattern recognition of odors in spoiled grain. The unique properties of neural networks have been shown to have significant potential for handling low-quality information. On reflection, this unique application is not so different from the problems encountered in classifying and handling hazardous wastes.

A simplified implementation of pyrolysis-EC has also been tested that uses a single sensor and a single catalytic filament. This drastically simplified system was still capable of distinguishing many organic chemicals. With fewer parts and lower power consumption, this simplified configuration may be suitable for selective hand-held vapor monitors.

Experimental Methods

Organochlorine sensor. The sensor was made by mounting a coil of platinum wire on a threaded base. A separate platinum wire is also mounted on the base and located axially within the coil. A mixture of lanthanum oxide, lanthanum fluoride, and a binder was applied to the coil. The coil was slowly heated with an electric current until a reaction occurred, forming the active material. The sensor is used by heating it to 550 °C with an electric current; conductivity is measured between the heating coil and the separate platinum electrode. When the sensor contacts the vapor of a chlorinated organic compound, the conductivity increases. A simple circuit can be used to provide a voltage output which is proportional to the concentration.

Permeation device. The permeation sampler consisted of a bundle of 0.025" o.d. dimethylsilicone tubing (Silastic, Dow-Corning) (Figure 1). The bundle could be placed in an aqueous sample containing dissolved organic or organochlorine compounds. A continuous flow of air was circulated through the lumen of the tubing, and organic material diffusing inward through the silicone membrane entered the gas phase. In a typical experiment, two permeators were used to provide separate reference and sample signals (Figure 2).

Pyrolysis-EC. The CPS-100 Toxic Gas Monitor has been described in several earlier publications (5-11); its configuration is diagrammed in Figure 3. The four sensors had platinum or gold working electrodes. For the grain odor experiments, the sensors were biased at differing oxidizing potentials, since reducing potentials gave very low or poor signals. A single rhodium pyrolysis filament was operated at 25, 450, 750, and 850 °C. The combination of four sensors and four temperatures gave an array of sixteen data points per analysis.

The apparatus for simplified pyrolysis-EC consisted of a single platinum filament and a single platinum-electrode gas sensor. A control circuit maintained the catalyst at any one of four preselected temperatures. The filament was enclosed in a Teflon-lined chamber of small volume through which the analyte gas was pumped at about 50 cc/min. The gas then passed through a short tube to the sensor. The experiments were controlled, and data gathered, by a commercial datalogger (Onset Computer Corp., N. Falmouth, MA).

Gas samples. Accurate samples of test compounds in vapor form were made by injecting measured volumes of the liquids into 40-liter Tedlar gas bags and filling with air pumped through a charcoal/Purafil filter. A flowmeter together with a stopwatch was used to determine the volume of air being pumped into the bag. Samples of permanent gases were made from standard mixtures obtained from commercial sources. Volumes of the standard mixtures and air were calculated and pumped into a sample bag, using the flowmeter and stopwatch to determine the volumes.

Samples from grain odors were generated by heating a sample of grain to 60 °C and flushing with a measured volume of air. The effluent air was passed through an ice trap to collect a "non-volatile" fraction and a liquid nitrogen trap to collect the "volatiles". The two fractions were run separately and in duplicate. Grain samples were obtained from Drs. L. Seitz and D. Saur of the USDA Grain Marketing Research Laboratory.

Results and Discussion

Organochlorine sensor. Typical responses of the sensor to different vapors in air are shown in Figure 4. The sensor was exposed to 100 ppm concentrations of chlorobenzene, benzene, and *n*-hexane. Only chlorobenzene caused a response. Of a series of compounds investigated, only HCl, and compounds containing carbon-chlorine and carbon-bromine bonds, gave a response (Table I). The response to concentration is essentially linear over at least four orders of magnitude.

Combined with the permeator device, the highly-selective organochlorine sensor was shown to respond rapidly to dissolved material. Figure 5 shows the response to chloroform in water at concentrations that dip below the part-per-million level. This sensor can be used to measure an organochlorine in groundwater, for example, without any sample preparation. Many sites, especially military bases, and areas such as Rockford, Illinois, where there is a large concentration of machine shops, have serious problems with chlorinated C2 compounds in the groundwater. In these cases, the nature of the compounds is generally known, and selectivity is not a concern. Nevertheless, the sampling procedure, sample preparation, and gas chromatography to determine these compounds is involved and expensive. The availability of a simple probe that can just be inserted into a groundwater sample will greatly reduce the number of laboratory analyses that need to be done. The silicone material is chemically resistant, and can be left in place for years. Particulates cannot enter the system. Lastly, and importantly, the permeator is very inexpensive.

Pyrolysis-EC: Grain Odors Only a few organic compounds will react directly with amperometric sensors under field conditions. On a typical, platinum-electrode sensor, we can detect alcohols, epoxides, and formaldehyde. We also detect many permanent gases, such as carbon monoxide and hydrogen sulfide. Among these gases that do react, there is no inherent selectivity. The use of different sensors and controlled pyrolysis, however, gives us extra degrees of freedom that can be used to achieve selectivity.

The grain odor problem is very instructive, even to an audience that is concerned with identifying individual hazardous compounds. Sensor-array-based methods, including the pattern-analysis methodologies used, treat mixtures no differently than single compounds; both give characteristic patterns which can be identified against a pattern made from the same mixture. The individual components of a mixture need not be identified.

Grains are presently classified by odor by a panel of trained inspectors. The results are necessarily subjective. More importantly, the subjective opinion is the **standard**; there is no point in telling a customer that a sample of grain is acceptable because a machine says so. If it smells bad, it smells bad. On the other hand, trained inspectors frequently disagree to a greater or lesser extent on both the category and degree of an odor (Table II). Attempts to identify specific compounds associated with the odors, using GC or GC/MS, have produced masses of data, but limited results (12, 13).

The data obtained on the CPS-100 was subjected to two different kinds of analysis. The first was an established method called **k-nearest neighbor** (KNN, ref. 5). The 16 data points acquired by the CPS-100 were treated as a vector in 16-dimensional space. Each known sample of grain produced a vector which could be associated with a particular odor category. The vectors from the unknown samples were tested against this library of known vectors by calculating the scalar distance between the unknown vector and each known vector in the library. All vectors were first normalized to constant length, to remove the concentration-dependent part of the information. The shortest distance is the identification (Figure 6).

The second method is the **neural network** (for general references, see 14, 15). This is a recently-developed method that has received so much "hype" that we were at first suspicious of it. However, its performance has been outstanding in this application, the moreso because we used a commercially-available packaged method (NeuroShell, Ward Systems Group, Frederick, MD), without really understanding the internal mechanics of the method. This is a very important feature of a method which may be used in the field by operatives with differing technical backgrounds.

Figure 7 shows the CPS-100 data, in histogram form, for "good" wheat samples. The patterns are very similar, in contrast with data showing some extreme samples (one "sour" (S3) and one "insect" (I3) odor) (Figure 8). A experiment using the older KNN method was run using a dataset derived from three grades of wheat samples. A library of vectors was prepared by averaging the signals for all runs on each sample of wheat. The scalar distances were calculated between all possible pairs of the original data set and each of the averaged vectors. A summary of the identifications is shown in Table III. We were very (pleasantly) surprised to find that those samples that are "misclassified" by the KNN algorithm are also those that the human inspectors did not agree on! Sample 42, for example, was voted "good" by two inspectors and "musty" and "COFO" by the other two. (COFO means "commercially objectionable foreign odor".)

Although KNN has shown good performance in past applications (5, 6, 8-11), it has some serious practical disadvantages. The greatest is that, when the sensors become aged or drift for other reasons, the complete training set must be remeasured.

A larger data set had been gathered by the time the work was begun with the neural nets. This data set had a peculiarity built into it: one of the sensors in the array went bad halfway through the measurements and was replaced. The data taken after that point gave noticeably different histograms.

The data set was arbitrarily divided into two groups. One group was used to "train" the neural network, a process requiring up to 150 hours on a 386-type computer. The actual classification process took seconds. Two tests were run on the optimized neural net. First was a test to confirm that the optimization process was complete. This was done by using the training set itself as unknowns. The rate of correct classification was 100%. Second, random, linearly-distributed errors were added to the data, followed by classification. The net tolerated 5% error without missing a correct classification. Added error of 10% and 15% caused a small amount of degradation (Table IV).

Having confirmed the robustness of the neural net, it was challenged using the reserved dataset. The net had not seen these numbers before; nevertheless the rate of correct classification was 65% (Table IV). This is low, although substantially better than random. Because the test conditions had changed during the measurements, we added another element to the data vectors to differentiate the measurements made before and after the sensor was changed. The numbers were arbitrary, 100 for the old sensor and 200 for the new. Using these 17-element vectors, the neural net was retrained. Now, the rate of correct classification of the reserved dataset jumped to 83%.

Pyrolysis-EC: Simplified Version This work is the result of a project to determine whether a greatly-simplified form of pyrolysis-EC would be useful for situations requiring limited selectivity. Figure 9 is a diagram of the patterns obtained for representative compounds in a typical experiment. The temperature of the catalyst is programmed for two minutes at room temperature, two minutes each at temperatures of 500, 600, 700, and 800 °C, and finally two minutes at room temperature again. The patterns that are obtained are distinct for many compounds. If your field problem is simply confirming the identity of the contents of a number of similar barrels of an unknown chemical, the pyrolysis-EC approach may in itself be sufficient, although most practitioners would feel more comfortable if it supplemented other field screening methods.

A table of distances for this limited configuration is shown in Table V. The smaller the number, the more similar the two compounds will appear for a given configuration of the experimental apparatus. This configuration gives very good identification of ethylene oxide in the presence of all but alcohols.

The pyrolysis-EC method has several advantages that are especially conducive to field work. It is suitable for portable instrument use; the components are shock-resistant and will operate in any orientation. They compact and lightweight, and the power requirements are small. They are also inexpensive.

Conclusions

1. A sensor has been developed and characterized that can identify chlorinated or brominated compounds in the vapor phase or, with the use of a permeable membrane, in dissolved form.

2. A combination of catalytic pyrolysis and electrochemical detection (pyrolysis-EC) can be used to distinguish unknown compounds with a modest degree of selectivity that may be adequate for many field applications.

3. Pyrolysis-EC data, combined with k-nearest neighbor and neural network classification methods, has been used effectively for such varied tasks as the classification of stored grains by odor, or the classification of waste chemicals by functional group (11).

4. The neural net can be made to adapt dynamically to instrument drift. In effect, it learns from experience.

4. Errors made by the classification methods correspond in a general way to errors made by human experts faced with similar ambiguities in the data.

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Table I. Sensitivities of the organochlorine sensor to several halogenated compounds.

Vapors	Concentration (ppm)	Response (x 10 mho/ppm)
C_3H_7Cl	125	0.024
C_3H_7Br	125	0.016
C_3H_7I	125	0.003
C_6H_5F	62.5	0.005
C_6H_5Cl	62.5	0.029
C_6H_5Br	62.5	0.020
C_6H_5I	125	0.003
C_2ClF_5	12.5	0.022

Table II. Subjective odor characterization of the grain samples used in our study.

SAMPLE No.	OMRL INSPECTORS				FGIS CONSENSUS	AVE INTENSITY
	DS	LS	KF	HM		
F41	C2	OKO	OKO	OKO	OK	0.5
F42	OKO	OKO	M1	C2	OK	0.7
F67	OKO	M1	OKO	OKO	OK	0.2
F78	OKO	OKO	M2	OKO	OK	0.5
F128	OKO	OKO	OKO	OKO	OK	0.0
F30	I3	I3	I3	I3	INSECT	3.0
F39	I2	C3	I2	C1	INSECT	2.0
F69	I1	I2	I2	M3	INSECT	2.0
F89	I3	I3	I2	S3	INSECT	2.7
N53	I2	S3	S2	S3	S3	2.8'
N166	S3	S3	S3	S3	S3	2.9'
N168	S2	S3	S2	S2	S3	2.6'

Table III. KNN classification of the USDA grain samples.

		Average of Known Vectors Good (128, 42, 67, 41)	 Insect (30, 39, 89)	 Sour (53, 166, 168)
"Unknown" Vectors	Good	128, 128, 42, 67, 67, 41, 41, 41, 41	42	42
	Insect	89	30, 30, 30, 39, 39, 89, 89, 89	30
	Sour	168	168, 168	53, 166, 166, 166, 168, 168

Table IV. Summary of the accuracy of the neural network algorithm for identifying vapors drawn from the wheat samples.

Sorghum <u>Data Set</u>	Accuracy of <u>Identification</u>	Wheat Samples <u>Data Set</u>	Accuracy of <u>Identification</u>
1. Original Data	100%	1. Total Data	100%
2. 5% Error added	100%	2. Train on 55% of Data set	65%
3. 10% Error Added	98%	3. Add channel for Test Conditions	83%
4. 15% Error Added	92%		

Table V. Distance matrices for a series of organic compounds. Table V-A is several concentrations of ethylene oxide; the concentrations are shown as the numbers in the symbols, e.g., ETO100 = 100 ppm. Table V-B shows the distances among the series of thirteen compounds. The Abbreviations are:

CHX - cyclohexane
ETE - ether
CLO - chloroform
FORM - Formaldehyde
ETO - Ethylene Oxide
ISO - isopropanol
KER - kerosene
STY - styrene
ETG - ethylene glycol
ACE - acetone
XYL - xylene
HAL - halothane
ETA - ethanol

TABLE V-A
Distance for Ethylene Oxide

	ETO100	ETO40	ETO20	ETO5	ETO5	ETO1
ETO100	0.00	0.31	0.28	0.22	0.25	1.02
ETO40	0.31	0.00	0.07	0.21	0.18	0.80
ETO20	0.28	0.07	0.00	0.21	0.16	0.82
ETO5	0.22	0.21	0.21	0.00	0.09	0.85
ETO5	0.25	0.18	0.16	0.09	0.00	0.80
ETO1	1.02	0.80	0.82	0.85	0.80	0.00

TABLE V-B

	CHX	ISO	ACE	ETE	XYL	KER	CLO	STY	FORM	HAL	ETG	ETO	ETA
CHX	0	1.57	0.19	1.76	1.02	1.07	0.69	1.44	1.74	2.09	1.52	1.73	1.95
ISO	1.57	0	1.42	0.44	0.76	0.62	1.49	0.46	0.31	0.72	0.4	0.62	0.81
ACE	0.19	1.42	0	1.59	0.85	0.91	0.55	1.27	1.58	1.93	1.35	1.55	1.77
ETE	1.76	0.44	1.59	0	0.82	0.74	1.53	0.41	0.2	0.59	0.3	0.25	0.38
XYL	1.02	0.76	0.85	0.82	0	0.34	0.88	0.45	0.85	1.27	0.55	0.75	0.98
KER	1.07	0.62	0.91	0.74	0.34	0	1	0.49	0.76	1.08	0.54	0.75	0.95
CLO	0.69	1.49	0.55	1.53	0.88	1	0	1.26	1.55	1.93	1.33	1.44	1.62
STY	1.44	0.46	1.27	0.41	0.45	0.49	1.26	0	0.45	0.93	0.12	0.37	0.63
FORM	1.74	0.31	1.58	0.2	0.85	0.76	1.55	0.45	0	0.61	0.34	0.41	0.56
HAL	2.09	0.72	1.93	0.59	1.27	1.08	1.93	0.93	0.61	0	0.84	0.79	0.73
ETG	1.52	0.4	1.35	0.3	0.55	0.54	1.33	0.12	0.34	0.84	0	0.3	0.55
ETO	1.73	0.62	1.55	0.25	0.75	0.75	1.44	0.37	0.41	0.79	0.3	0	0.27
ETA	1.95	0.81	1.77	0.38	0.98	0.95	1.62	0.63	0.56	0.73	0.55	0.27	0

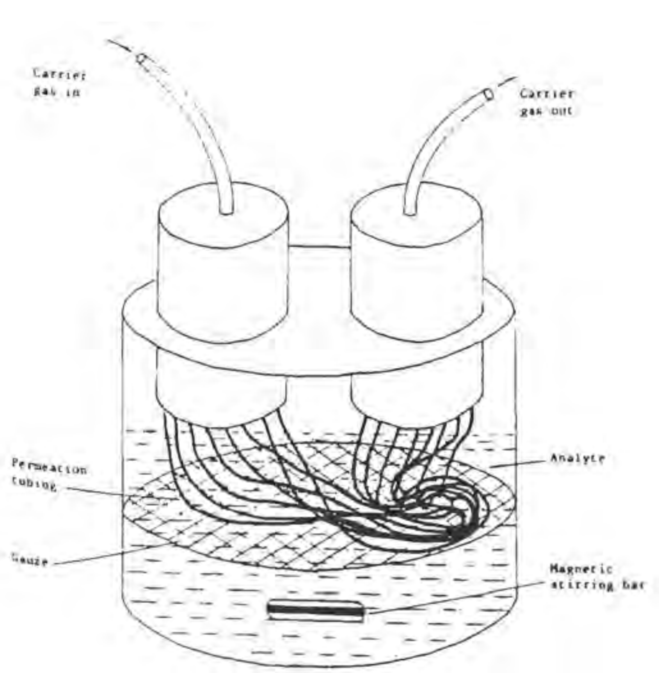


Figure 1. Permeation apparatus used to extract organochlorines from water.

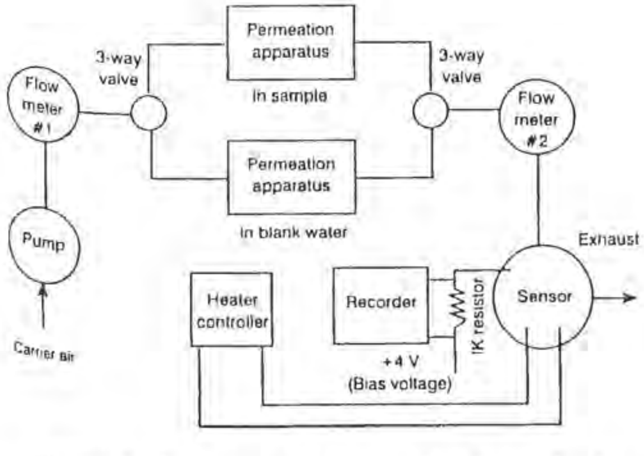


Figure 2. Experimental apparatus for selective analysis of aqueous chlorinated hydrocarbons using a separate reference permeator.

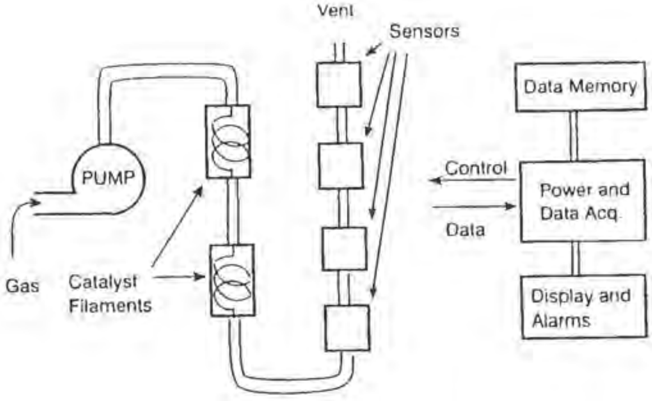


Figure 3. Configuration of the CPS-100 Toxic Gas Analyzer, fitted with four electrochemical sensors and two catalyst filaments.

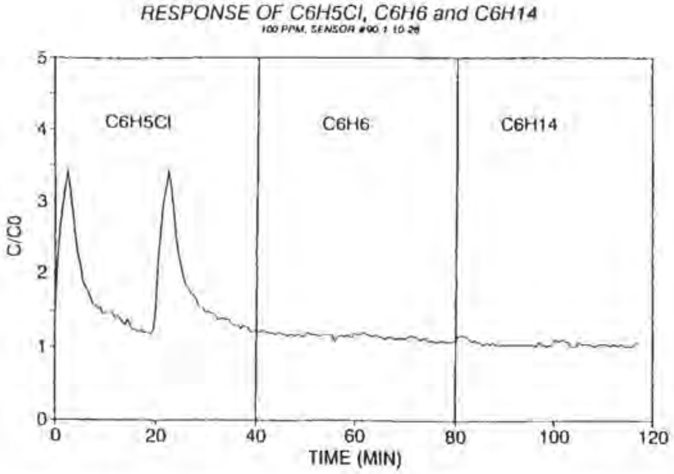


Figure 4. Response of the organochlorine sensor to chlorobenzene, benzene, and hexane.

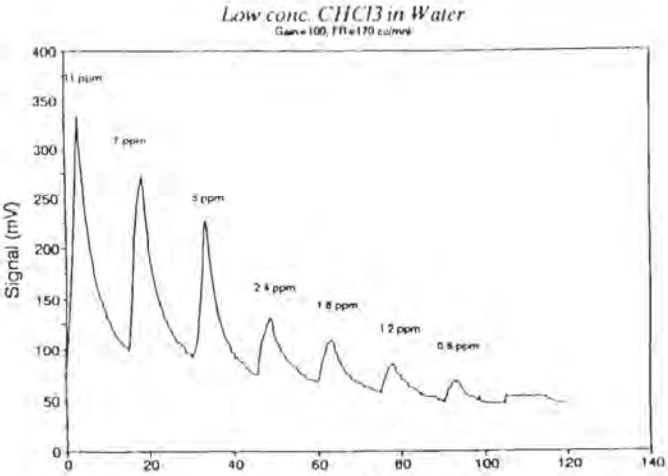
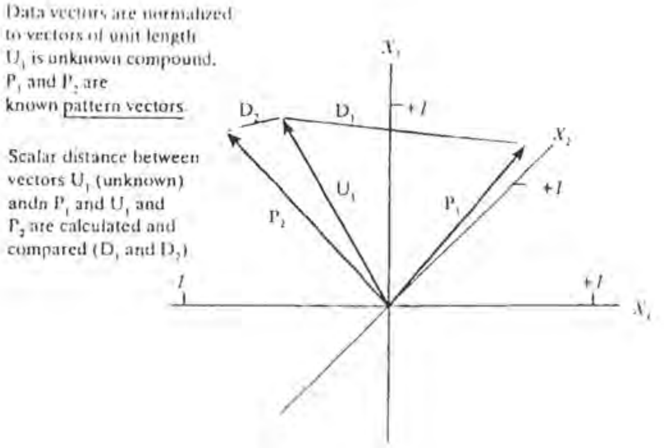


Figure 5. Response of the organochlorine sensor to decreasing concentrations of chloroform.



Data vectors are normalized to vectors of unit length U_1 is unknown compound. P_1 and P_2 are known pattern vectors.

Scalar distance between vectors U_1 (unknown) andn P_1 and U_1 and P_2 are calculated and compared (D_1 and D_2)

Figure 6. Schematic representation of the KNN pattern recognition method in 3-dimensional space. P1 and P2 are library patterns for known compounds, and U1 is the vector for an unknown. The distances from U1 to P1 and P2 are calculated and compared.

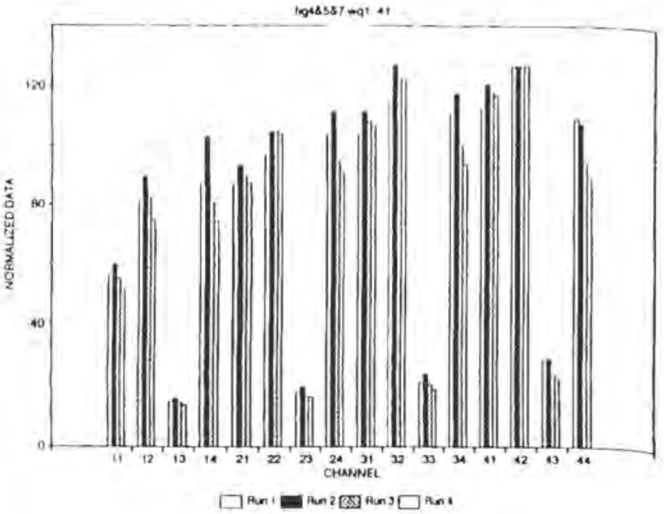


Figure 7. Histogram of normalized responses of the CPS-100 to four samples of "good" grain.

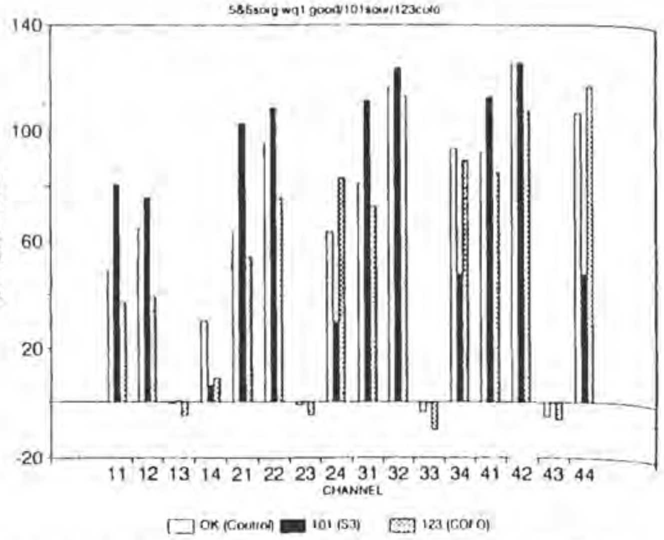
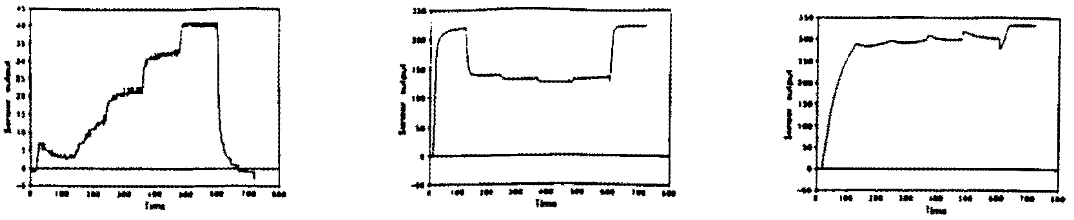
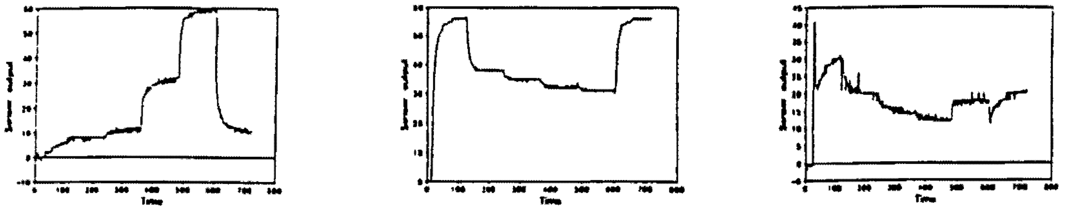


Figure 8. Normalized responses of the CPS-100 to "good" (OK), sour (S3), and COFO grain.



Chloroform Isopropanol Ethylene Oxide



Acetone Ethanol Halothane

Figure 9. Responses of the simplified pyrolysis-EC apparatus to six different chemicals. In this experiment, the catalyst filament was programmed in 2 minute steps at room temperature, 500, 600, 700, and 800 degrees, and room temperature again.

DISCUSSION

GORMAN BAYKUT: My question is about the chemical analysis with these sensors. I'm not talking right now about the wheat vapor. But in terms of real chemical analysis, you must know the compounds you are going to analyze, otherwise you can't do the analysis because you need training. You can't analyze the unexpected compounds, am I right?

WILLIAM BUTTNER: The way the CPS 100 Program was originally envisioned, you had to install the library vectors of potential compounds. If you were going to look at TCE, there had to be a library vector associated with the TCE. On the other hand, these arrays are not totally selective in response. The response to TCE was similar to PCE, that is, tetrachloroethane. You could therefore identify classes of compounds. But you are right. You have to have some idea of the type of vapors present. A totally unknown situation will still give some ambiguity in your analyses.

GORMAN BAYKUT: But I think even though your software is powerful, you need a training period for every compound. How about the mixtures? If you analyze the mixtures will there be a problem?

WILLIAM BUTTNER: Mixtures are a problem for this type of system. Certain types of mixtures are well behaved. Gasoline, for example, is a mixture of many types of compounds, but it behaves as a single class.

GORMAN BAYKUT: I'm referring to the cracker. You have a thermal cracker in front of the electrochemical sensor areas. Sometimes you have a mixture of two or three compounds, or five, or seven and they react in the cracker. You get different answers, and the correlation is not linear.

WILLIAM BUTTNER: What you're referring to are the reaction products of the thermal catalysis that result from mixtures being exposed to the sensors. Yes, you are right. There is frequently a nonlinear response. The reaction products frequently do react with each other. That's a comment relevant to many field screening techniques. In some mixtures that factor is a little less significant. If you do generate very reactive compounds, for example from chlorinated compounds TCE, you do get a nonlinear response. That is a problem. This instrument was designed to look at single vapors, maybe not necessarily positively identified, but single vapors.

STEVEN KARR: I wondered if you've given any thought to applying fuzzy logic algorithms to this problem as opposed to neural networks?

WILLIAM BUTTNER: The neural network was a six-month program that we tried on the SBIR (we've just finished Phase I). To stay within the time constraints, we stuck to simple systems. We are investigating other neural network software packages and other identification algorithms. We will certainly consider fuzzy networks.

EDWARD POZIOMEK: Have you tried any real-world environmental samples with the system.

WILLIAM BUTTNER: I had a program through Savannah River to monitor for TCE emissions out of their stripping tower, as part of their groundwater clean up. Initially the results were very encouraging. The analyses that I measured were compared back to groundwater samples as measured at an independent laboratory. They were comparable in value. The unfortunate thing is that these amperometric sensors did not behave truly reversibly to chlorinated compounds, and that after a period of time their response factor, their sensitivity, would degrade and ultimately their response would die completely. For that reason it was determined that these types of sensor systems would not be applicable for the problems associated with Savannah River Laboratory. This was before this chlorine selective sensor was developed. It could potentially have application down there.

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