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Digital Sensors and Sensor Systems: Practical Design

Sergey Y. Yurish

The goal of this book is to help the practicians achieve the best metrological and technical performances of digital sensors and sensor systems at low cost, and significantly to reduce time-to-market. It should be also useful for students, lectures and professors to provide a solid background of the novel concepts and design approach.

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Data Mining Approach to Polymer Selection for Making SAW Sensor Array Based Electronic Nose

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Abstract: In this paper, a simple application of principal component analysis and hierarchical clustering methods of classical data mining has been demonstrated for making selection of polymer coatings for surface acoustic wave (SAW) sensor array. The database consists of thermodynamic solvation parameters of the prospective polymers and the target vapors. The linear-solvation-energy-relationship (LSER) has been used to calculate partition coefficients from the solvation parameters. The partition coefficient data for various vapor-polymer combinations is then arranged as a data matrix taking the polymers for instances (rows) and the vapors for variables (columns). Selection of polymer subset for optimal discrimination of target vapors from background interferents has been made by analyzing the principal component score and load plots. A simulation study for detection of trinitrotoluene (TNT) and dinitrotoluene (DNT) explosive vapors camouflaged in the background of 29 interferent organic vapors originating from varied sources such as soil, vegetation, body odor, and indoor and outdoor industrial/commercial environments has been carried out. The paper demonstrates that the application of data mining methods for the selection of polymeric sensor coatings could prove prudent in terms of reducing system complexity, cost and development time. *Copyright © 2012 IFSA.*

Keywords: Polymer selection, Data mining, SAW sensor array, Electronic nose, TNT/DNT vapor detection.

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1. Introduction

Electronic nose is a sensor array system that mimics working of mammalian odor sensing organ [1-4]. The array sensors are sensitive to odorant molecules in vapor phase to varying degrees. Upon exposure to an odor sample, the sensor array generates a response pattern that is analyzed by pattern recognition methods to identify the odor. Today, electronic nose technology has become an important development pursuit to fulfill various application needs such as health monitoring through body odor analysis, food products monitoring for quality and freshness, indoor air quality and fire safety monitoring, industrial process and environment monitoring, explosive detection for homeland security, and so on [5-11].

The sensors are very basic to generating information about target chemicals in the form of electrical signal that are often acquired in digital format for subsequent data processing [12, 13]. The information coding in sensor outputs the following processing for extraction of vapor identities are two crucial aspects of electronic nose operation. They need different kinds of expertise. The design and development of sensors need special materials, which could interact with odorants in selective manner. The sensor array design needs a set of chemical selective materials that offers sufficiently broad variation in selectivities across target odorant molecules. Individual sensors in the array when functionalized with different materials of this set map odorants selectivity patterns into array response patterns. The odor identities are thus coded into sensor array response patterns. The data processing objective is to decode this response pattern and create odors mathematical signature. A number of reviews and recent books have covered rationale, methods, status of technology and applications of various types of electronic noses [1-13]. Excellent discussion is however given in some earlier publications [14-20].

The challenges of sensor array making and data processing for pattern recognition are usually handled by different sets of researchers and developers, it is obvious though that the electronic nose system performance could be optimized only through understanding and exploitation of implicit mutual dependencies. For example, pattern recognition algorithms could be designed having better efficiency if vapor induced sensor response models could reveal mathematical relations between identity making chemical parameters and sensors output. This would help in selecting right data transformation and classification approaches. A model based analysis of polymer functionalized surface acoustic wave (SAW) sensors [21] and subsequent elaboration in [22] has demonstrated this. The logarithmic scaling of input data suggested by thermodynamic sensor model in [21] substantially improves interclass dispersion in feature space created by independent component analysis (ICA) and principal component analysis (PCA), classification efficiency of a neural network classifier. The studies involving tin-oxide gas sensors and composite conducting polymer sensors also support a similar situation [23, 24]. In an unpublished study, the present authors also found that a power scaling of outputs from these sensors as prompted by the nonlinear dependence of sensor responses on vapor concentration improves classification rate of a neural network classifier. The sensor model suggested processing strategy is to be contrasted with the abstract mathematical procedures based on statistical and functional considerations.

In the present work, we advance the application of data processing capabilities to the sensor array design stage. The motivation is to see if we can mine the existing database on vapor-polymer interactions to select an optimal set of sensor coatings for some specific target detection. The selected polymers must provide maximum discrimination for target vapors against interferent vapors in ambient. As a case study, we consider the detection of explosive trinitrotoluene (TNT) vapor based on polymer coated SAW sensor array. The ambient is visualized by considering application situations such as landmine detection, bomb detection in market place and frisking cargo and human for explosive threat detection. A number of volatile organic compounds (VOCs) likely to be present in ambient air are considered as interferents. They may have varied origins such as soil and vegetation, body odor, vehicular emission and commercial activities. The vapor-polymer solvation database for those polymers which are available commercially is utilized in this study. We apply the well-known classical data mining methods PCA and hierarchical clustering for selection of an optimal subset of polymers from a large set which were shortlisted heuristically their solvation parameters. A number of laboratory synthesized polymers reported by different groups, but not available commercially, are excluded from the present analysis. This is done with the purpose to exploit commercial resources only for any cost effective development of electronic nose system. The validation of selection is done by generating synthetic sensor array response data and pattern recognition analysis. The details are elaborated in the sections below.

2. Background

In the past, search for optimum set of polymers for SAW sensor array coatings has progressed in two directions. In one, new materials are developed through polymer chemistry route either by polymer synthesis or by functionalizing backbone of available polymers with vapor selective groups, or by combining both [25-35]. In the other, based on knowledge base about chemical solubility and interactions in various vapor-polymer combinations, prospective polymers are shortlisted from the list of available polymers, sensor arrays are made by selecting them heuristically in short groups, evaluating their responses for detection of target vapors by pattern recognition methods, and selecting the best performing among them either empirically or by employing some selection algorithm [14, 36-40]. The first approach mainly enriches the list of candidate polymers to choose from. The second approach is actually what has been practiced in most of the earlier studies. The methodologies and developments is these directions are very well covered in a review [37] and a book [38]. The rationale of polymer selection based on measurements of sensor responses and multivariate data processing is nicely discussed in one of the earliest publications [14]. Most commonly, the principal component analysis (PCA) and clustering methods are used. However, in some studies, search and optimization approaches based on genetic algorithm (GA) [39] and Fisher information [40] are illustrated.

It is not difficult to realize that selection of an optimal set of polymers by making sensor arrays and analyzing responses is costly and time-consuming process. The interaction between vapors and polymers in various combinations are extensively studied based on thermochemical sorption-desorption experiments such as gravimetric and chromatography, and substantial database on solvation, plasticization and viscoelastic properties is available [32, 36, 41-47]. As mentioned before, this paper is set to examine if this database could be mined to arrive at some theoretical design of sensor array that optimally meets target requirements. The validation and fine-tuning, of course, would be done by performing real experiments. However, a prior short listing based on some intelligent data processing of existing data may substantially reduce time and cost for developing specific electronic nose systems.

We consider a specific case of SAW sensor array design for detection and identification of trinitrotoluene (TNT) vapor in presence of potential interferent vapors in gaseous ambient. A SAW sensor is a polymer coated SAW device (delay line or resonator) which is employed as frequency control element in an oscillator circuit. The sorption of odorant vapor species into the polymer coating affects propagation of surface acoustic waves which in turn produces change in the frequency of the oscillator circuit. The sensor output is the vapor induced change in the oscillator frequency. The details of SAW sensor operation can be found in [38]. The SAW sensor array comprises a number of SAW sensors in which individual sensors are coated with different polymers. The latter are selected to be different in selectivities towards target group of chemical species for detection. The selection of polymer coatings is crucial to the working of SAW sensor array based electronic nose. The motivation of this study is to explore the available database about vapor-polymer interactions to determine which set of polymers would provide maximum discrimination of target vapors (TNT in our case) against ever present background of ambient vapors. For this, we apply well-known classical data mining methods, PCA and hierarchical clustering on solvation database. We make a selection and validate it by generating sensor array responses based on a well-established SAW sensor model [48]. Further details are elaborated in the following sections.

3. Data Mining for Polymer Selection

The database consists of quantitative information about chemical nature of vapor molecules and polymers. The geneses of vapor-polymer interactions lie in molecular structure and electronic configurations of both the vapor molecules and the polymer matrix. These interactions are modeled as composed of certain linearly independent subinteractions, which individually contribute to the vapor sorption in a polymer matrix. The complimentary chemical properties like hydrogen bond acidity of vapor molecules and hydrogen bond basicity of polymer matrix induced chemical affinity that favors solvation or sorption. In selecting polymers, an important point that is kept in mind is that the sensors are required to be reversible, in addition to being selective and sensitive. That is, the vapors should desorb with ease upon removal of vapors from the sensor cell. This can happen only if the chemical interactions are weak. Therefore, the polymers in which with weak hydrogen bonding, polar, nonpolar and dispersive interactions are dominant are the potential candidates for selection. The polymers having strong covalent and ionic interactions are not suitable for making electronic nose sensors.

The sorption by weak chemical interactions is usually modeled by an empirical equation which relates vapor partitioning into polymer as sum of several terms, each corresponding to an interaction process. This equation is known as LSER (linear solvation energy relation) [42, 49-51], and is written as

$$\log K = c + rR_2 + s\pi_2^* + a\sum\alpha_2^H + b\sum\beta_2^H + l\log L^{16} \tag{1}$$

where K is called the partition coefficient. It is defined as $K = C_P / C_V$, where C_P and C_V are concentrations of analyte vapor molecules in the polymer and the vapor phases respectively in thermodynamic equilibrium. The sensor loading (hence the signal magnitude) is determined by the value of K. In this equation, each term on the right hand side corresponds to a specific solvation interaction. Except the first term, each term is a product of two parameters, one represents the vapor molecules and the other represents the polymer matrix. These are called solvation parameters of the respective species. The parameters c, r, s, a, b and l characterize solvation characteristics of the polymer (called solvent), and R_2, π_2^*, $\sum\alpha_2^H$, $\sum\beta_2^H$ and $\log L^{16}$ characterize complementary solvation characteristics of the vapor (called solute). The r and R_2 are measures of interaction via dispersion forces; s and π_2^* measure solvation due to dipole interactions; a measures hydrogen bond basicity of the polymer and $\sum\alpha_2^H$ measures hydrogen bond acidity of the vapor; b measures hydrogen bond acidity of the polymer and $\sum\beta_2^H$ measures hydrogen bond basicity of the vapor; l and $\log L^{16}$ measure combined effects of dispersion interaction and cavity formation in a reference matrix called hexadecane; and c is a regression constant that quantitative representation to any residual effect that is not covered by the other terms. Also note that the LSER equation is written for $\log K$, that is logarithm to the base 10.

Different polymers have different sets of solvation parameters. Therefore, an analyte vapor with its own specific set of solvation parameters would generate different outputs from a sensors array coated with multiple polymers. The data processing methods attempts to estimate the set of vapor solvation parameters or some unique representation of them from the measurement of sensor array response. The set is taken to be the mathematical signature of the analyte vapor. In order that the electronic nose system differentiates mathematical signatures of different vapor species both the selection of polymer set that encodes as diverse information about analytes as possible and the data processing algorithms that are able to extract vapor signatures accurately and efficiently are important.

The database consists of tables of values of solvation parameters for various vapor molecules and polymers. The strategy for mining this database is to create a data matrix consisted of *K*-values calculated by using the LSER equation and solvation parameters for different vapors of interest in rows, and the potential polymers in columns. Then, extract polymers signatures in terms of vapors by applying the principal component analysis. In principal component space, the polymers having similar properties will be closer, and those having distinctly diverse properties will be farther. By studying the distribution of polymers in principal components space one can select a subset of those polymers which are most diverse or dissimilar from each other. With these polymers as sensor array coatings, one can expect to encode attributes of vapors signature in sensors output in most differentiable manner.

3.1. Target Vapors and Interferents

As mentioned earlier, we take up here a case study of detection and identification of TNT explosive vapors camouflaged in ambient background containing several volatile organic compound (VOC) vapors of varied origins. The TNT is a very common explosive used either alone, or mixed with higher explosives such as RDX and HMX, or in high energy explosives as ignition material. The vapor detection of explosive materials requires their vapor pressure to be adequate for introducing detectable amount in ambient. The partial vapor pressures at ordinary temperatures of some common explosive materials are: DNT (dinitrotoluene) in ppm (parts per million) range, TNT (trinitrotoluene) in ppb (parts per billion), RDX (research development explosive ─ cyclotrimethylene trinitramine) and PETN (Pentaerythritol tetranitrate) in ppt (parts per trillion) range, and HMX (high melting explosive ─ octahydro-tetranitro tetrazocine) ppq (parts per quadrillion) in range [52-54]. The DNT is always present in TNT as manufacturing impurity. Therefore, even though as impurity, since DNT vapor pressure is nearly 3 orders of magnitude larger than TNT, headspace over TNT charge contains DNT vapors in comparable concentration [55]. A polymer selection exercise for TNT detection, therefore, must target DNT detection as well. The TNT vapor detection may be useful for detection of other high explosives (RDX, PETN and HMX) also, because TNT is invariably present in high explosive devices as igniter and its vapor pressure is much higher than theirs is.

The reliable detection of explosives vapor signature or vaporprints at such low concentrations is extremely difficult. This difficulty grows many folds in real field situations as the ambient is loaded with several VOCs from different origins. For example, ambient air over landmines will carry VOCs originating from soil and vegetation, ambient around a human body carrying hidden explosives will carry VOCs of body odor, or ambient of a busy market place where an explosive device is suspected will carry mixed VOCs from body odor, vehicular emission and other commercial activities of the place [56, 57]. Keeping these in view, a set of 29 likely representative interferent VOCs were selected based on the studies published in [58-81]. This is shown in Table 1. Another factor that influenced the selection of these interferents is the availability of their solvation parameters [41-47]. Several of these originate from more than one source. Therefore, they are arranged roughly according to their chemical category and likely sources of origin as indicated. Wherever available, their saturated vapor pressures are also indicated [82]. The solvation parameters of the selected vapors were collected from the reports in [41-46], and are presented in Table 2.

3.2. Potential Polymers

Most of the published work on TNT/DNT vapor sensing by polymeric sensors is summarized in [41-43]. A list of prospective polymers was prepared by using the information in these reports. Keeping in mind whether their solvation parameters are known, and whether they are commercially available, a list of 22 polymers is presented in Table 3. Of them, the first 10 polymers were found listed in the catalog of some commercial suppliers. Of the rest, individual researchers had synthesized some, and the origin of some could not be traced. They were assumed not available commercially. As said before, we intend to seek optimum set of polymers for TNT detection from those available commercially. Therefore, further analysis is based on only the first 10 polymers in Table 3.

Table 1. Target explosive vapors and interferent gases from different origins.

Target vapors [52-55]	
TNT	Common explosive, 4.5×10^{-6} mmHg @ 20 ^{0}C
DNT	Impurity in TNT, 1.1×10^{-4} mmHg @ 20 ^{0}C
Interferent vapors [58-82]	
Water	Universal interferent
Acetaldehyde	Body odor, tobacco leaves and smoke, wood, combustion of natural gas and oil 52 mmHg @ 37^{0}C
Hexanal	Body odor, wood, vegetation, building materials, residential, work place, 10 mmHg @ 20 ^{0}C
Heptanal	-
Octanal	2 mmHg @ 20^{0}C
Nonanal	0.26 mmHg @ 20^{0}C
Benzaldehyde	4 mmHg @ 45^{0}C
Ethanol	Body odor, vehicular emission, plants, combustion of wood, 73 mmHg @ 20 ^{0}C
Hexanol	Body odor, vegetation, 1 mmHg @ 25.6 ^{0}C
Phenol	Body odor, residential and workplace, automobile exhaust, combustion of wood
Cresol	Body odor, automobile exhaust, combustion of wood
Benzyl alcohol	Body odor, interior paints, 13.3 mmHg @ 100 ^{0}C
Benzene	Body odor, workplace and residential environment, unburnt petro products, combustion of wood, 166 mmHg @ 37.7 ^{0}C
Toluene	22 mmHg @ 20 ^{0}C
Acetone	Body odor, wood pellets, 185.5 mmHg @ 20 ^{0}C
Isoprene	456 mmHg @ 20 ^{0}C
Acetic acid	body odor, plants, automobile exhaust , 11.4 mmHg @ 20 ^{0}C
n-Hexanoic acid	Body odor, incineration plants, 0.18 mmHg @ 20 ^{0}C
n-Octanoic acid	Body odor, automobile exhaust, road dust, tire debris, organometallic breaks, leaf surface of plants, 1 mmHg @ 78 ^{0}C
n-Nonanoic acid	< 0.1 mmHg @ 20 ^{0}C
n-Decanoic acid	15 mmHg @ 160 ^{0}C
n-Undecanoic acid	-
Caffeine	Drugs of abuse
Procaine	
Nicotine	
Diazepam	
Barbital	
Paracetamol	
Butalbarbital	

3.3. K-matrix, PCA and Polymer Selection

The equilibrium partition coefficient for each vapor-polymer combination is obtained by using the LSER equation and the solvation parameters data in Tables 2 and 3. The $\log K$ values are shown in Table 4.

The $K_{31\times10}$ matrix obtained after taking antilog is the data matrix for our analysis. The equilibrium vapor loading into a polymer is given as $C_P = KC_V$, proportional to *K*-value. Each row in Table 4 represents a vapor as a set of 10 *K*-values associated with different polymers. If a 10-element sensor array is constructed by coating these polymers (each on a separate SAW platform), and if the sensor outputs are linearly related to loadings, then the Table 4 can be interpreted as 31×10 data matrix of vapors sensing.

Table 2. Thermodynamic solvation parameters for target explosive and interferent vapors [41-48].

Chemical vapor	Solvation parameters				
	R_2	π_2^*	$\sum\alpha_2^H$	$\sum\beta_2^H$	$\log L^{16}$
TNT	1.43	2.23	0	0.61	7.85
DNT	1.15	1.6	0	0.47	6.26
Water	0	0.45	0.82	0.35	0.26
Acetaldehyde	0.208	0.67	0	0.45	1.23
Hexanal	0.146	0.65	0	0.45	3.357
Heptanal	0.14	0.65	0	0.45	3.865
Octanal	0.16	0.65	0	0.45	4.361
Nonanal	0.15	0.65	0	0.45	4.856
Benzaldehyde	0.82	1	0	0.39	4.008
Acetone	0.179	0.7	0.04	0.56	1.7
Ethanol	0.246	0.42	0.37	0.48	1.49
Hexanol	0.21	0.42	0.37	0.48	3.61
Phenol	0.805	0.89	0.6	0.3	3.766
Benzyl alcohol	0.803	0.87	0.33	0.56	4.221
Benzene	0.61	0.52	0	0.14	2.79
Toluene	0.601	0.52	0	0.14	3.33
Cresol	0.84	0.86	0.52	0.3	3.766
Isoprene	0.31	0.23	0	0.1	2.101
Acetic acid	0.265	0.65	0.61	0.44	1.75
n-Hexanoic acid	0.174	0.6	0.6	0.45	3.92
n-Octanoic acid	0.15	0.6	0.6	0.45	5
n-Nonanoic acid	0.132	0.6	0.6	0.54	5.55
n-Decanoic acid	0.124	0.6	0.6	0.45	6.09
n-Undecanoic acid	0.1	0.6	0.6	0.45	6.64
Caffeine	1.5	1.6	0	1.33	1.3632
Procaine	1.14	1.67	0.32	1.36	1.9767
Nicotine	0.865	1.44	0	0.9	1.371
Diazepam	2.308	2.11	0	1.15	2.07
Barbital	1.03	1.14	0.47	1.18	1.374
Paracetamol	1.06	1.78	1.09	0.81	1.172
Butalbarbital	1.03	1.14	0.47	1.18	1.6557

A principal component analysis on *K*-matrix would generate a feature space defined by eigenvectors of K^TK covariance matrix [83]. If this set of polymers were able to capture different interaction attributes of vapors (solvation parameters) in sufficiently different proportions, then the loadings generated by them would be different. Hence, a linear PCA must succeed in creating feature space where different vapors occupy separate regions. However, if some of the polymers generate similar or overlapping information then they are either redundant or ineffective in producing class separation. The polymer selection is to eliminate similar (or not adequately dissimilar) polymers from a large list of prospective polymers so that the best subset that produces largest separation in the feature space is obtained. If we take transpose of *K*-matrix then each row would represent a polymer in terms of 31 vapors as variables. The principal component analysis on $K_{10\times 31}^T$ will yield feature space defined by eigenvectors of KK^T, in which different polymers occupy separate regions if they are characteristically different from the perspective of vapors. However, if the vapors do not discriminate enough between some of them, overlaps would occur. A single polymer from each overlapping group would generate nearly the same information about vapors as all in the group together. Therefore, only one polymer from each overlapping group may be selected, and the rest can be treated as redundant. Thus, if we find well-separated groups of polymers in the feature space created by KK^T – eigenvectors, we can select one polymer from each group and prepare a shortlist. However, ambiguity remains about which polymer from a group must be selected, and whether there is need for further elimination. These issues can be resolved by analyzing principal components score plots and load plots complimentarily.

Table 3. Solvation parameters of potential polymers for TNT/DNT sensors [41-44].

Polymer			**Solvation Parameters**						
			c	*r*	*s*	*a*	*b*	*l*	
1.	Polyisobutylene	PIB	-0.77	-0.08	0.37	0.18	0.00	1.02	
2.	Polyepichlorohydrin	PECH	-0.75	0.10	1.63	1.45	0.71	0.83	
3.	Poly-trifluoropropyl-methylsiloxane	OV202	-0.39	-0.48	1.30	0.44	0.71	0.81	Commercial
4.	75% Phenyl-25%methyl-polysiloxane	OV25	-0.846	0.177	1.287	0.556	0.440	0.885	
5.	Poly-ethylenimine	PEI	-1.580	0.495	1.516	7.018	0.000	0.770	
6.	Poly-dimethylsiloxane	PDMS	0.18	-0.05	0.21	0.99	0.10	0.84	
7.	Poly-methyl cynopropylsiloxane	PMCPS	-0.12	0.02	1.65	2.71	0.38	0.72	
8.	Poly-methyl phenylsiloxane	PMPS	-0.20	-0.03	0.97	1.11	0.10	0.86	
9.	Fomblii-ZDOL	ZDOL	-0.49	-0.75	0.61	1.44	3.67	0.71	
10.	Poly-vinyl propionate	PVPR	-0.57	0.67	0.83	2.25	1.03	0.72	
11.	Poly-methyl-amino-propylsiloxane	PMAPS	-0.01	-0.23	0.97	1.99	0.24	0.83	
12.	Poly-methyl (isopropylcarboxylicacid) siloxane	PMiPCAS	0.13	-0.16	0.79	2.36	0.28	0.77	
13.	Poly-methyl (2-carboxy (D-valinyl-tert-butylamide) propyl) siloxane)	CSVAL	0.02	0.05	0.23	2.22	0.46	0.85	Non-commercial
14.	Fluoropolyol	FPOL	-1.21	-0.67	1.45	1.49	4.09	0.81	
15.	Poly-vinyltetradecanal	PVTD	-0.59	-0.02	0.74	2.44	0.22	0.92	
16.	Poly-ethylene maleate	PEM	-1.65	-1.03	2.75	4.23	0.00	0.87	
17.	Poly-vinyl propionate	PVPR	-0.57	0.67	0.83	2.25	1.03	0.72	
18.	Poly-bis cynopropyl-siloxane	SXCN	-1.63	0.00	2.28	3.03	0.52	0.77	
19.	Hexafluoro-2-propanol-substituted polysiloxane	SXFA	-0.08	-0.42	0.60	0.70	4.25	0.72	
20.	Alkylaminopyridyl-substituted polysiloxane)	SXPYR	-1.938	-0.189	2.425	6.780	0.000	1.016	
21.	Poly 4-hexafluoroisopropanol-styrene	P4V	-1.33	-1.54	2.49	1.51	5.88	0.90	
22.	-	SXPHB	-0.85	0.18	1.29	0.56	0.44	0.89	

Table 4. Equilibrium log *K* calculated by using LSER equation and solvation parameters tabulated in Tables 2 and 3 for 10 polymers and 31 vapors.

Vapor	**Polymer**									
	PIB	PECH	OV202	OV25	PEI	PDMS	PMCPS	PMPS	ZDOL	PVPR
TNT	7.9477	9.9765	8.6142	9.4928	8.553	7.2318	9.4719	8.7322	7.61	8.5193
DNT	6.1152	7.5025	6.5423	7.1637	6.235	5.7639	7.2288	6.7481	5.793	6.5198
Water	-0.1907	1.6368	1.0149	0.5732	5.0572	1.3397	3.1649	1.4053	2.4344	2.1962
Acetaldehyde	0.7159	1.7033	1.697	1.3397	0.4858	1.3885	2.0463	1.5465	2.2875	1.4746
Hexanal	2.883	3.4299	3.4236	3.1853	2.0626	3.1741	3.5435	3.3581	3.832	2.9479
Heptanal	3.4016	3.8509	3.838	3.6339	2.4508	3.6011	3.9091	3.7952	4.1971	3.3096
Octanal	3.9059	4.2646	4.2301	4.0764	2.8426	4.0167	4.2666	4.2212	4.5343	3.6801
Nonanal	4.4116	4.6745	4.6359	4.5127	3.2188	4.433	4.6228	4.6472	4.8933	4.0298
Benzaldehyde	3.6226	4.5655	4.0398	4.3048	3.4281	3.7547	4.5804	4.2313	3.782	4.0969
Acetone	1.2159	2.2755	2.2263	1.8597	1.1595	1.8416	2.5838	2.036	3.1226	2.0217
Ethanol	0.9521	2.0732	1.7484	1.4737	2.9224	1.9218	2.8358	1.9401	2.934	2.3431
Hexanol	3.1174	3.8292	3.4829	3.3435	4.537	3.7044	4.3615	3.7644	4.4662	3.8454
Phenol	3.4442	4.99	3.9081	4.2404	7.2783	4.1141	5.8161	4.5739	4.088	5.0786
Benzyl alcohol	3.8525	5.1279	4.3174	4.5813	5.7025	4.2509	5.4778	4.6722	4.9658	5.0485
Benzene	2.2194	2.5737	2.3525	2.462	1.6586	2.6163	2.8122	2.6995	1.8644	2.4233
Toluene	2.7709	3.021	2.7942	2.9383	2.0699	3.0704	3.2008	3.1642	2.2546	2.8061
Cresol	3.4159	4.8286	3.8171	4.1635	6.6887	4.0268	5.5505	4.455	3.9283	4.8971
Isoprene	1.4333	1.4707	1.533	1.4083	0.5399	1.9876	1.8164	1.8307	1.2765	1.4443
Acetic acid	1.3441	2.9854	2.3261	2.119	5.1651	2.4212	4.0381	2.6486	3.4434	3.2327
n-Hexanoic acid	3.5445	4.6885	4.0652	3.9578	6.6449	4.2291	5.4929	4.459	5.0442	4.6805
n-Octanoic acid	4.648	5.5825	4.9515	4.9093	7.4647	5.1375	6.27	5.3885	5.829	5.442
n-Nonanoic acid	5.2104	6.1011	5.4695	5.4325	7.8792	5.6094	6.6998	5.871	6.5633	5.9186
n-Decanoic acid	5.7619	6.4846	5.8469	5.8694	8.2911	6.0544	7.0543	6.3267	6.6224	6.2094
n-Undecanoic acid	6.3248	6.9387	6.3039	6.3519	8.7027	6.5176	7.4498	6.8004	7.0309	6.5893
Caffeine	1.0925	4.0838	3.0185	3.2703	2.6378	1.7191	4.0369	2.6124	5.21	4.1144
Procaine	1.8305	5.1564	3.9413	4.0308	5.2838	2.5869	5.4655	3.5769	6.5292	5.1239
Nicotine	1.092	3.4606	2.8163	2.7697	2.0869	1.6808	3.6024	2.4399	4.0161	3.1189
Diazepam	1.9375	5.4547	3.7384	4.616	4.3551	2.3615	5.3351	3.6727	4.7563	5.4026
Barbital	1.0555	3.8709	2.7551	2.8	5.0145	2.1054	4.493	2.6962	5.4158	4.3285
Paracitamol	1.1954	5.3858	3.4192	3.6321	10.1952	2.6454	6.9437	3.7936	5.1752	5.7482
Butalbarbital	1.3428	4.1047	2.9833	3.0493	5.2314	2.342	4.6958	2.9385	5.6158	4.5313

By doing PCA on K^T with eigenvectors of KK^T as basis, it is found that the 10 polymers appear in the main list in 4 separate groups in the feature space. Fig. 1 shows this. It consists of two principal components score plots, one in PC1-PC2 plane, Fig. 1(a), and the other in PC2-PC3 plane, Fig. 1(b). In Fig. 1(a), one group consists of 6 polymers (PDMS, ZDOL, PIB, PVPR, OV202 and PMPS), second has 2 polymers (OV25 and PMCPS), and third and fourth groups have only one polymer in each (PECH and PEI respectively). Note that the PECH is well separated from the others in PC2 direction, and PEI is well separated from the others in PC1 direction. Therefore, PECH and PEI clearly stand out as obvious selection as they are capable of generating two different type of information about the vapors. Actually, the vapors see them differently. In other words, these two polymers would capture two independent intrinsic dimensionalities of the 31 vapors. The remaining two groups are seen to be very close to PECH in PC1 direction, to PEI in PC2 direction. Therefore, by including a polymer from these groups is not expected to produce significantly different information in PC1-PC2 plane than that by PECH and PEI. However, if we look in the third direction, Fig. 1(b), it is found that PMCPS from group 2 stands out from the rest. It means PMCPS captures information about a third intrinsic dimensionality of the vapors. Note that its eigenvalue is very small in comparison to the first two components hence it appears insignificant. However, sometimes, small independent information is of great help in discriminating vapors with little chemical differences. That means, PMCPS can be included as the third selection. The load plots shown in Fig. 2 further support this argument. It can be seen that PECH, PEI and PMCPS generate maximum loads in three mutually orthogonal directions. Therefore, it is concluded that these 3 polymers are the best subset selection from the original list of 10 for TNT/DNT discrimination.

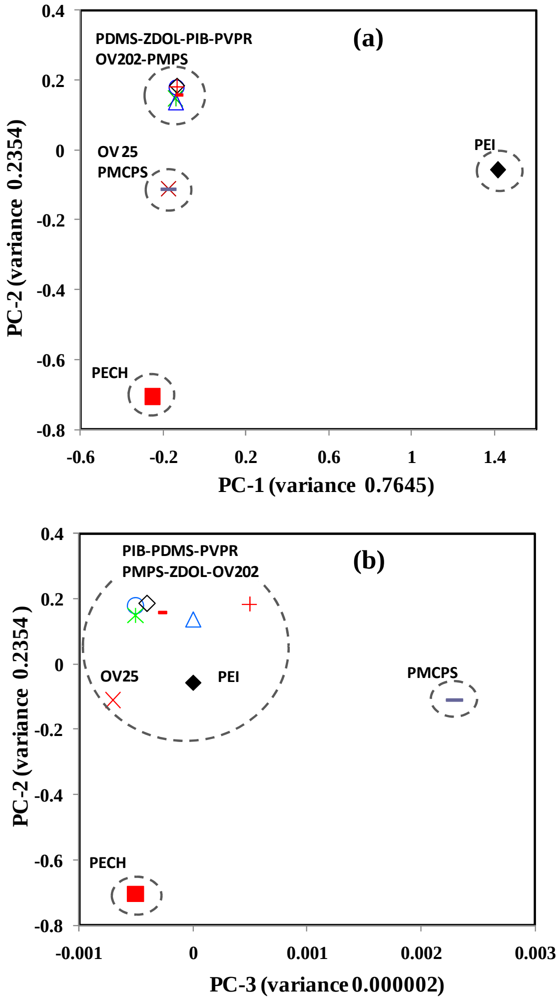

Fig. 1. Principal component score plots of *K*-matrix based on eigenvectors of KK^T (see text).

3.4. Hierarchical Clustering

The clustering methods are often used to sort out objects into groups based on some measure of similarity among them. The divisive hierarchical clustering has been used earlier to make selection of SAW sensors for hazardous vapor detection [16]. Application of clustering methods involves defining some measure of similarity between objects as recorded in the values of measured variables [84]. A simple measure of similarity often used in the literature is Euclidean distance. A hierarchical clustering analysis on the transposed data matrix K^T by using Euclidean distance measure between polymers and single-link algorithm yields the dendogram shown in Fig. 3.

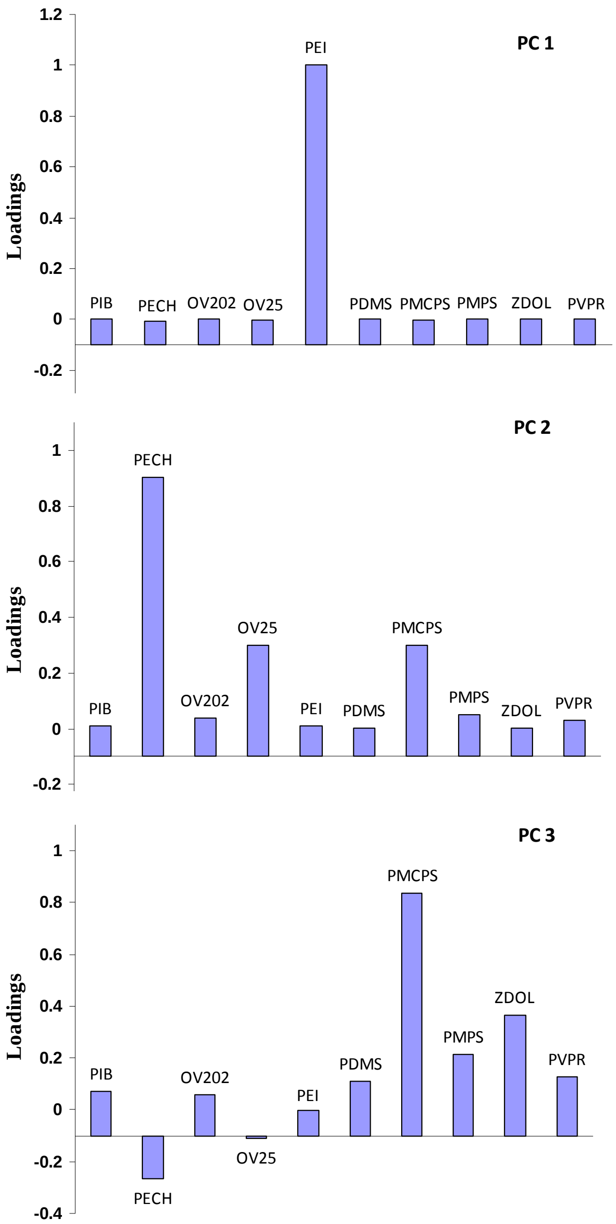

Fig. 2. Loadings of different polymers on principal components.

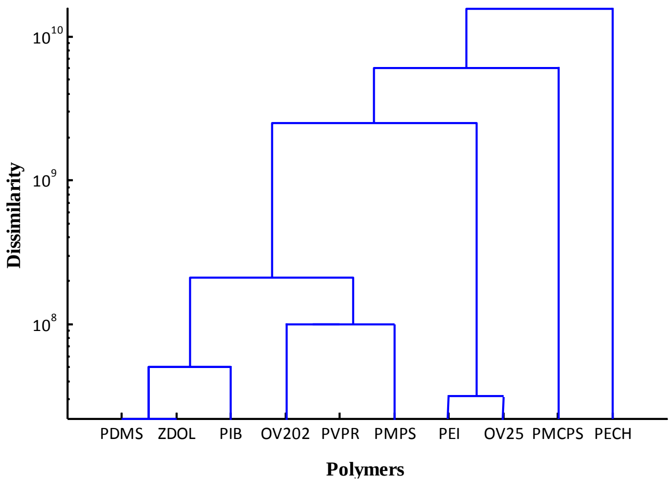

Fig. 3. Hierarchical dendogram of ten commercial polymers that were short-listed as prospective coating materials for SAW sensors.

Recall that in the interpretation of hierarchical clustering dendogram the most dissimilar objects join at the highest level on Euclidian distance measure (y-axis here). It can be noted that the polymers appear in groups similar to those seen earlier in the PCA score plots. However, the group compositions slightly differ. Here, PEI and OV25 appear as a highly similar group as they are at low level. However, they both are quite dissimilar from PMCPS and PECH as they join latter at high level. This dendogram suggests that PECH, PMCPS, and one of PEI and OV25 must be selected to be the most dissimilar polymer subset. However, it does not provide any basis for making a preferred choice between PEI and OV25. Moreover, note that groupings in hierarchical dendogram depend on the definition of similarity measure. Any refinement in similarity definition and/or some data preprocessing before clustering may alter the appearance of groups in dendogram.

4. Validation

4.1. SAW Sensor Array and Data Generation

In order to validate above described polymer subset selection we generate synthetic SAW sensor array response matrices by using a well-established sensor model [48]. Exposure to all 31 vapors is considered. A comparative study of three sensors arrays of different sizes is made. The first sensor array consists of 10 sensors each coated with a different polymer from the original set. The second sensor array consists of 3 sensors each coated with a different polymer from the selected subset of 3 polymers, namely, PECH, PEI and PMCPS. The third sensors array consists of only 2 sensors, one coated with PECH and the other with PEI. The third combination is included for comparison to examine the influence of PMCPS on vapor discrimination. We saw that the eigenvalue associated with the third eigenvector is extremely small in comparison to the first and second eigenvectors (Fig. 1), and we associated the former to PMCPS in view of the loadings in Fig. 2. Therefore, it appears that PMCPS role must be insignificant. The analysis below clarifies this point.

To calculate SAW sensors output for a given vapor exposure we used a simplified analytical representation of the full model in [48]. The latter has complex parametric dependencies on different material constants. The derivation of the analytical relation and its validity are described in detail in [85]. According to this relation the SAW sensor frequency change due to polymer coating is given as

$$\frac{\Delta f_p}{f_0} \cong -\omega h \rho_p \left[(c_1 + c_2 + c_3) - \frac{c_1 + 4c_3}{\rho_p v_0^2} G' + \frac{1}{2} (\omega h)^2 \rho_p (c_1 + c_3) \frac{G'}{|G|^2} \right] \tag{2}$$

where f_0 is the SAW oscillator frequency before polymer coating and Δf_p is the change in frequency due to polymer coating. The other symbols denote, $\omega = 2\pi f_0$ angular frequency, h polymer thickness, ρ_p polymer mass density, $G = G' + iG''$ polymer complex shear modulus where real part G' represents storage modulus and imaginary part G'' represents loss modulus, $|G|^2 = G'^2 + G''^2$, v_0 velocity of SAW propagation on free surface without coating, and c_1, c_2 and c_3 are material constants whose values depend on the piezoelectric SAW substrate and direction of surface wave propagation.

For the present study we consider SAW substrate to be STX quartz crystal having material constants $v_0 = 3.158 \times 10^5$ cms^{-1}, and $c_1 = 0.013 \times 10^{-7}$, $c_2 = 1.142 \times 10^{-7}$ and $c_3 = 0.615 \times 10^{-7}$ in units of cm^{2}sg^{-1}. We assume that nominal operating frequency of the uncoated SAW oscillators is

$f_0 = 200\,\text{MHz}$. The other sensor parameters associated with the polymer coatings are summarized in Table 5. The sensor output due to vapor sorption in polymer films will be obtained from the same relation (2) by calculating the additional change in frequency due to vapor sorption. This can be obtained by replacing ρ_p by $\rho_p + C_P$ in equation (2) where $C_P = KC_V$ is the change in polymer density due to vapor sorption. By subtracting the frequency change due to polymer coating (Δf_p) from that due to combined effect of vapor sorption and polymer coating (say Δf_v) one obtains the sensor output $\Delta f = \Delta f_v - \Delta f_p$.

Table 5. Polymer parameters used in the SAW sensor array response calculation.

Polymer	**Dominant solvation interactions**	**Glass transition temperature (^{0}C)**		**Film thickness (nm)**	**Mass density (g/cm^3)**		**Shear moduli (dyne/cm^2)**		
							$G' \times 10^7$	$G'' \times 10^7$	
PIB	Nonpolar	-71	[87]	98	0.918	[93]	800	800	[96]
PECH	Dipolar and hydrogen bond basic	-22	[87]	56	1.360	[93]	10	1	[97]
OV202	Dipolar	-70	[88]	72	1.252	[93]	2	5	
OV25	Dipolar	-30	[88]	78	1.150	[93]	2	2	
PEI	Strong hydrogen bond basic	-23	[89]	86	1.050	[93]	5	1	
PDMS	Nonpolar and hydrogen bond acidic	-123	[87]	91	0.98	[94]	1.5	8	[98]
PMCPS	Dipolar and hydrogen bond basic	-123	[90]	90	1.00	[90]	82	2	
PMPS	Nonpolar and hydrogen bond basic	-28	[88]	81	1.115	[95]	20	1	
ZDOL	Hydrogen bond acidic	-126	[91]	50	1.800	[93]	2	5	
PVPR	Hydrogen bond basic	-36	[92]	89	1.010	[93]	100	0.01	

Note: The unreferenced values are assumed to represent the polymer shear moduli keeping in view their glass transition temperatures.

The output from the three sensor arrays mentioned above were calculated for all 31 vapors at 30 concentration levels. In order to make the synthetic data appear more realistic, an additive Gaussian noise source was also included. That is, the sensors output were actually calculated as $\Delta f = (\Delta f_V - \Delta f_P) + \Delta f_{noise}$ where Δf_{noise} denotes the frequency fluctuation due to a Gaussian noise source. The mean and standard deviation of the noise source were taken to be 30 Hz and 50 Hz respectively to represent a typical SAW oscillator with ppm (part per million) level stability.

The 31 vapors make diverse motley of chemicals whose vapor pressures vary over a wide range. Therefore, 30 samples of each vapor were generated by incrementing their concentrations in unit step from 1 to 30 but at different scales. For low vapor pressure explosives TNT and DNT the scale is ppt (parts per trillion), for moderate vapor pressure drugs of abuse (caffeine, procaine, nicotine, diazepam, barbital, paracetamol and butalbarbital) and acetaldehyde the scale is ppb (parts per billion), and for all the rest the scale is ppm (parts per million). The vapor concentrations were converted from the parts by volume to g/cm^3 for use in Eq. (2) at normal temperature and pressure conditions. The range of concentration scales were selected after looking vapor data of these chemicals in [52-55, 58-82]. Thus the synthetic data matrices obtained for the sensor arrays 1, 2 and 3 are of sizes 930×10, 930×3 and 930×2 respectively with sensors in columns and vapor samples in rows.

4.2. Data Processing

The data analysis presented here is based on the principal component analysis. A preprocessing procedure has been implemented on the raw synthetic data before doing PCA. The said procedure is based on two recent analyses presented in [21] and [22]. It consists of data normalization, logarithmic scaling, mean centering and dimensional autoscaling steps in succession. The data normalization is done with respect to both the vapors concentration and the polymers thickness, and is implemented by dividing sensors output by vapor concentration (C_V) and frequency shift due to polymer coatings (Δf_p). The logarithmic scaling is to take logarithm of the normalized data $\Delta f \leftarrow \log(\Delta f / C_V \Delta f_p)$ and redefine the data matrix. The mean-centering and dimensional autoscaling are implemented by column. That is, by defining column mean as $\overline{\Delta f} = (1/N)\sum_{i=1}^{N} \Delta f_i$ and standard deviation as $\sigma = \sqrt{(1/N)\sum_{i=1}^{N}(\Delta f_i - \overline{\Delta f})^2}$ where the summation runs over the number of samples in a column, the data is transformed according as $\Delta f \leftarrow (\Delta f - \overline{\Delta f})/\sigma$ [86]. Finally, the principal component analysis of the preprocessed data matrices corresponding to all the three sensor arrays is done. Fig. 4 and Fig. 5 show the PC score plots from this analysis.

From a comparison of Fig. 4 (a, b) with Fig. 4(c, d) it can be clearly seen that the three sensor array based on selected polymer subset (PECH, PEI, PMCPS) separates the target TNT/DNT vapors from the rest. With all the 10 original polymers, the features overlap so much that no vapor class is separated, Fig. 4(a, b). In PC1-PC2 plane, however two major groups appear which consist of several vapor species. In comparison, the 3-element sensor array reveals hidden structures of data. Not only the TNT/DNT vapor classes are discriminated against background, some of interferent compounds are also separated as distinct group, Fig. 4(c, d). The results from 2-element sensor array based on PECH and PEI is shown in Fig. 5. Qualitatively, the results look similar to that in Fig. 4(c). However, a scrutiny reveals that by including the third polymer PMCPS in the sensor array makes quantitative impact by increasing interclass separations. The importance of PMCPS can be realized by comparing Fig. 4(b) and (d). It is clear how because of this the vapors are dispersed in PC3 direction.

5. Discussion

Development of microelectronic sensor system for detection of TNT vapor signature by sniffing air over suspect luggage, cargo or person is among high priority objectives in sensor research today. The favorable features that drive development of this technology are the high sensitivity and selectivity, fast response and reversibility, small size and portability, rugged and low cost of microsensors. The later features are the result of a mature SAW chip technology, low power sensor electronics, and compatibility with high volume production tools and techniques. The sensitivity, selectivity, response time and reversibility are however critically dependent on the selection of polymers, and the post sensing data processing. As mentioned before, empirical selection of sensors by fabrication and evaluation of sensor array in different combinatorial groups of polymers necessitate a large amount of experimentation and one by one selection or elimination of good or bad polymers. This involves large time and expenses. If the set of prospective polymers could be short-listed a priori by some method based on the basis of existing knowledge or data about usefulness of these polymers, the process of optimal sensor array development can be expedited, and can be made more flexible to suit specific applications. This will substantially reduce the development cost; and will also allow tuning of different set of polymers for different target applications. The approach presented here and the results in this paper clearly demonstrate this. The set of three polymers that were selected for TNT and DNT detection from a list of 10 commercially available polymers based on PCA and Hierarchical Clustering could successfully discriminate these vapors against 29 interferent gases of various origins. The validation based on synthetic data generation is quite reliable for SAW sensor array technology because the SAW sensor model used is an experimentally established model and the thermodynamic data taken is widely used reliable source. In future, as more polymers become available and the data bases are further enriched this approach will become more effective.

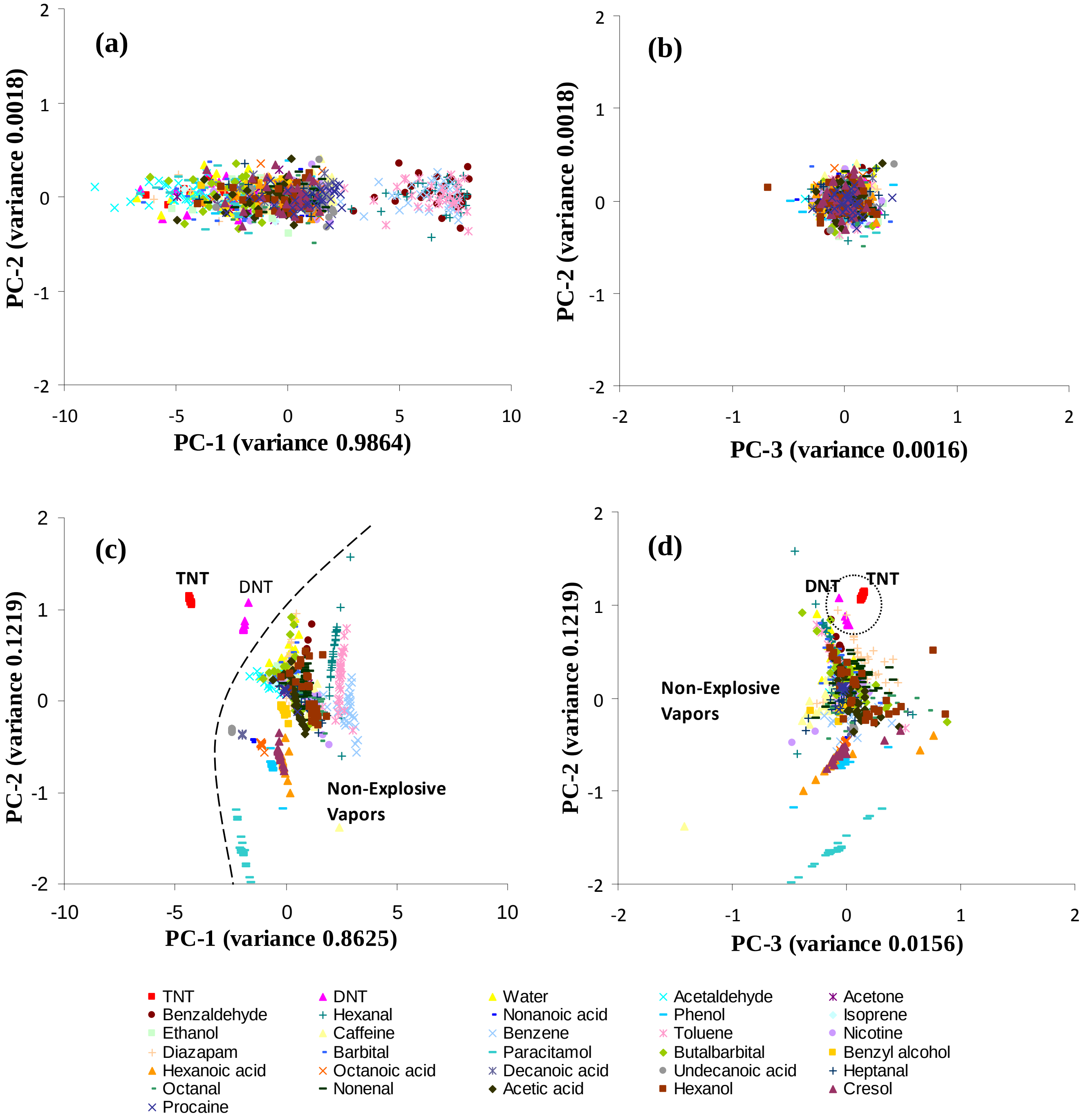

Fig. 4. Principal component score plots of SAW sensor array response for detection of TNT and DNT vapors in presence of 29 interferent vapors. The plots in (a) and (b) are based on the 10-element sensor array that uses all the 10 short-listed polymers. The plots in (c) and (d) are based on the 3-element sensor array that uses the selection subset of three polymers (PECH, PEI and PMCPS).

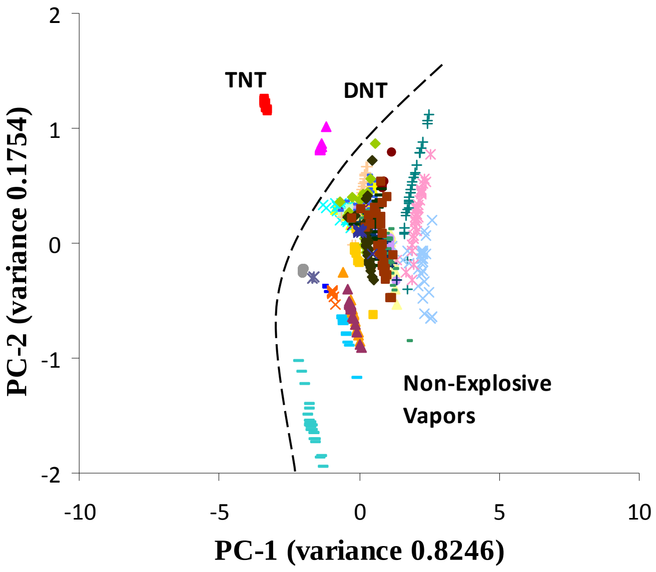

Fig. 5. Principal component score plots of 2-element SAW sensor array response based on PECH and PEI polymers.

The present analysis opens up another possibility that a large sensor array coated with diverse polymers targeting broad range of detection could be housed in one instrument and different subsets of sensors can be marked a priori for seeking detection of different target vapor classes, cross validation of results from one subset by that from another, and also fusion of results from different subsets for making the system more robust and reliable. The methods used in the present analysis are simple methods of classical data mining. The PCA assumes that the data variables are Gaussian and the hierarchical clustering is based on Euclidean distance metric. Both these methods assume the data space to be linear. This approach however could extended for nonlinear data spaces by using algorithms based on different assumptions such as non-gaussianity methods like independent component analysis [21] and kernel methods like the support vector machine [99].

6. Conclusion

Similar to the feature selection in a pattern recognition problem, it is shown in this paper that principal component analysis of vapor-polymer partition coefficient data could be used for selection of the most important polymers for making a sensor array for some specific vapor identification problem. This has been by treating the polymers as identification targets and the analyte vapors as sensors. The individual clusters in PCA generated feature space represent groups of polymers that are alike, that is, group of those that produce correlated information. Therefore, only one polymer from each group must be sufficient to define a sensor in the array. A polymer from each well-separated cluster will therefore capture most diversity of the target vapors. The simulation and analysis results presented in the paper amply support this. The artificial data generated in these simulations is based on an established SAW sensor model and real thermodynamic data of vapor-polymer solvation. Therefore, the sensor array design suggested by this approach could be trusted to be reliable. The case study of TNT and DNT vapor detection in the presence of 29 ambient interferent vapors of varied origins is presented. Starting from a set of 10 commercially available polymers shown in Table 3, which have substantial partitioning abilities for TNT, DNT and ambient interferent vapors, the present analysis short-listed three polymers: PECH, PEI and PMCPS. The interferents represented diverse backgrounds from human body odor, drugs of abuse, soil and vegetation to indoor and outdoor environment. The selection process has been validated by analyzing artificial data generated by a 3-element SAW sensor array coated with the selected polymers. The array responses are calculated by using an established

SAW sensor theory, and by incorporating an additive Gaussian noise source. From the analysis of synthetic data it is shown that the present selection successfully separates TNT and DNT vapors from interferents in PCA generated feature space. In conclusion, this study demonstrates the utility of data mining methods for making polymer selection for SAW sensors based electronic nose development.

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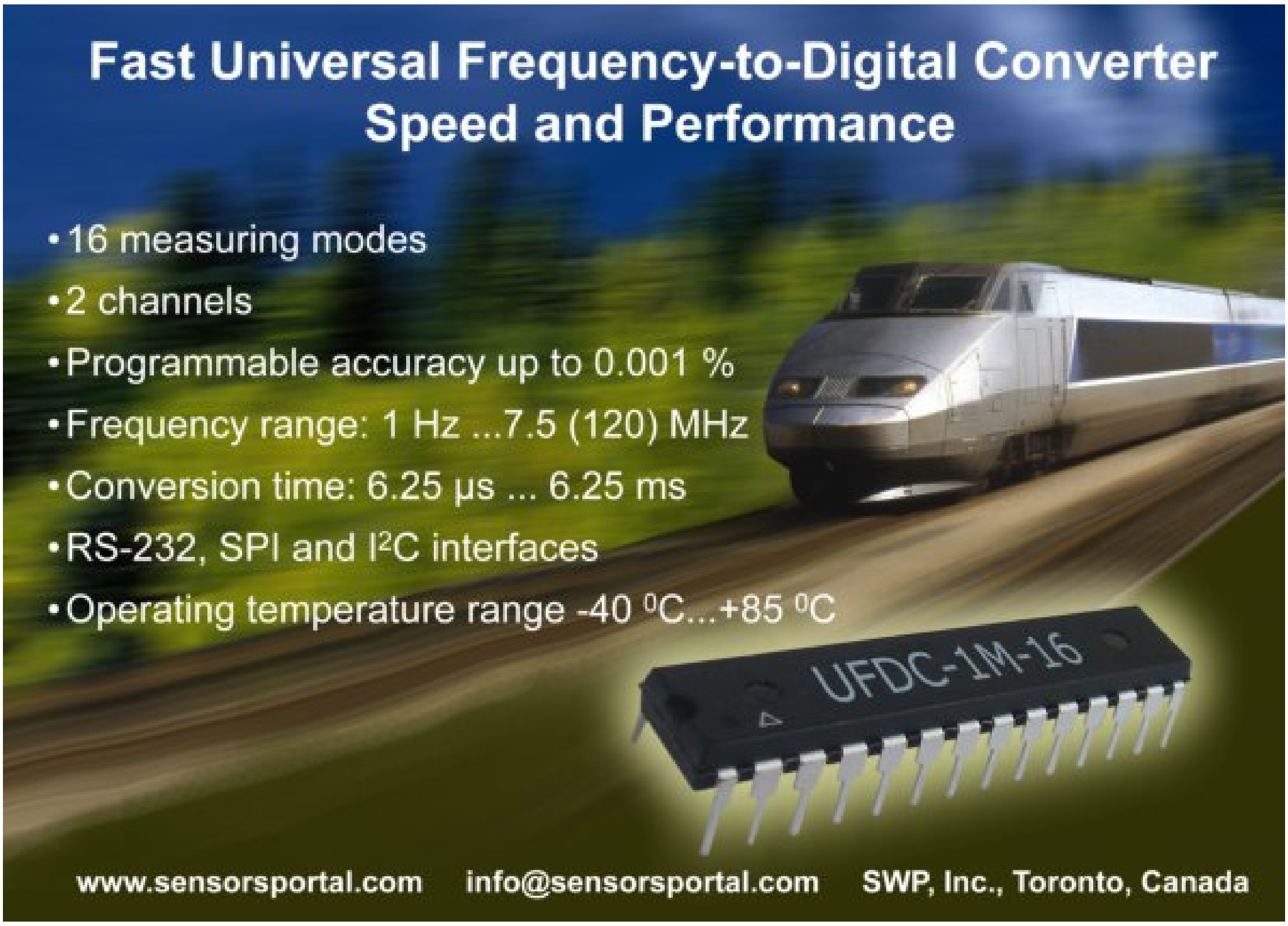

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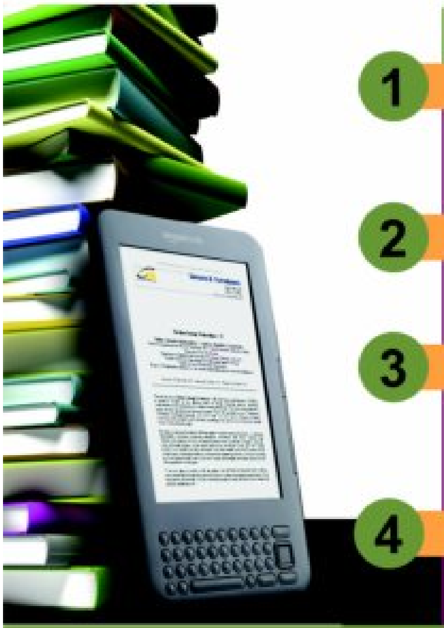

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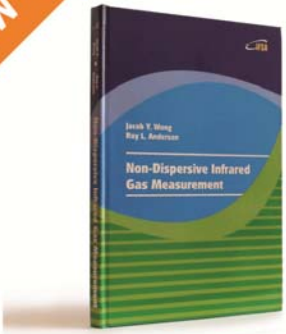

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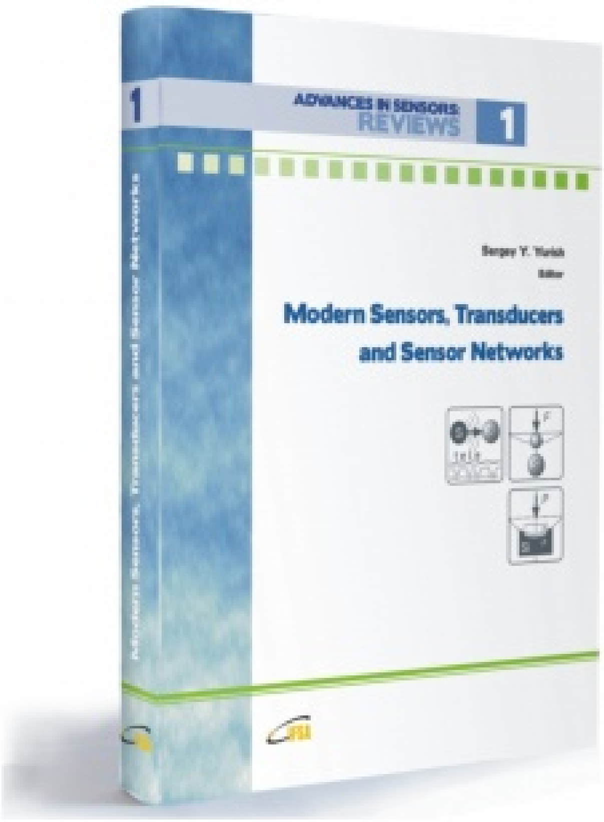
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