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Contents

Volume 126
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Research Articles

Human Heat Generator for Energy Scavenging with Wearable Thermopiles <i>Vladimir Leonov</i>	1
Fabrication of a Highly-sensitive Acetylcholine Sensor Based on AChOx Immobilized Smart-chips <i>M. M. Rahman</i>	11
Development of Pressure-Temperature Integrated Multifunction Sensor Using Piezo-Resistive Element <i>Palash K. Kundu, Gautam Sarkar and Chandan Dutta</i>	19
Prototype for Managing the Wheelchair Movements by Accelerometry <i>Daniel Alves Fusco, Alexandre Balbinot</i>	31
Design of an Automatic Path Finding Wheelchair with Intelligent Guidance System <i>Apratim Majumder, Niladri Banerjee, Shikha Nayak and B. Chakraborty</i>	42
Design and Manufacture an Ultrasonic Dispersion System with Automatic Frequency Adjusting Property <i>Herlina Abdul Rahim, Javad Abbaszadeh Bargoshadi, Sahar Sarrafi Ruzairi Abdul Rahim</i>	52
A Fusion Approach to Feature Extraction by Wavelet Decomposition and Principal Component Analysis in Transient Signal Processing of SAW Odor Sensor Array <i>Prashant Singh and R. D. S. Yadava</i>	64
Development of a Simple Traffic Sensor and System with Vehicle Classification Based on PVDF Film Element <i>D. R. Santoso, Abdurrouf, L. Nurriyah</i>	74
Practical Investigation of an Acoustic Encoder <i>Mohammad A. Alia, Mohammad Al-Khedher, Mazouz Salahat</i>	85
A Novel Method to Balance Inverted Pendulum by Angle Sensing Using Fuzzy Logic Supervised PID Controller <i>Sanjeev Kumar, Ashutosh K. Agarwal, Arpita Gupta, Himanshu Tripathi, Prachi Mohan Kulshrestha</i>	92
An Integrated Expert Controller for the Oven Temperature Control System <i>Nagabhushana Katte, Nagabhushan Raju Konduru, Bhaskar Pobbathi, and Parvathi Sidaraddi</i>	101
Implementation of PID Controller in MATLAB for Real Time DC Motor Speed Control System <i>Manjunatha Reddy H. K., Immanuel J., Parvathi C. S., P. Bhaskar and L. S. Sudheer</i>	110
Applying Time Series Analysis Model to Temperature Data in Greenhouses <i>Abdelhafid Hasni, Zouaoui Chikr-el-Mezouar, Belkacem Draoui and Thierry Boulard</i>	119

Growth Factor Inhibiting PKC Sensor in E-coli Environment Using Classification Technique and ANN Method

T. K. Basak, T.Ramanujam, S. Jeybalan, Madhubala Bhatt, Deepali Garg, Richa Garg

125

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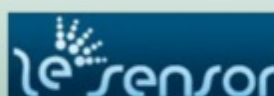
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A Fusion Approach to Feature Extraction by Wavelet Decomposition and Principal Component Analysis in Transient Signal Processing of SAW Odor Sensor Array

Prashant SINGH and R. D. S. YADAVA

Sensors & Signal Processing Laboratory, Department of Physics, Faculty of Science,
Banaras Hindu University, Varanasi 221005, India
Tel.: +91-542-2307308, fax: +91-542-2368390
E-mail: p8singh@gmail.com, ardius@gmail.com, ardius@bhu.ac.in

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Abstract: This paper presents theoretical analysis of a new approach for development of surface acoustic wave (SAW) sensor array based odor recognition system. The construction of sensor array employs a single polymer interface for selective sorption of odorant chemicals in vapor phase. The individual sensors are however coated with different thicknesses. The idea of sensor coating thickness variation is for terminating solvation and diffusion kinetics of vapors into polymer up to different stages of equilibration on different sensors. This is expected to generate diversity in information content of the sensors transient. The analysis is based on wavelet decomposition of transient signals. The single sensor transients have been used earlier for generating odor identity signatures based on wavelet approximation coefficients. In the present work, however, we exploit variability in diffusion kinetics due to polymer thicknesses for making odor signatures. This is done by fusion of the wavelet coefficients from different sensors in the array, and then applying the principal component analysis. We find that the present approach substantially enhances the vapor class separability in feature space. The validation is done by generating synthetic sensor array data based on well-established SAW sensor theory. *Copyright © 2011 IFSA.*

Keywords: SAW electronic nose, Wavelet decomposition, Feature extraction, Transient signal analysis, Odor sensor array, Information fusion.

1. Introduction

The surface acoustic wave (SAW) chemical sensor array based electronic nose is an extensively researched and developed approach of vapor detection and identification. The development of highly

sensitive electronic noses is important for a variety of application areas ranging from detection of explosives and chemical weapon agents, environmental pollutants, disease biomarkers in body odor and degradation of food and beverages to quality control of tea, coffee, cosmetics, fragrance etc. [1-6]. The operational paradigm of an electronic nose mimics working of human smell sensing organ. An array of chemical selective vapor sensors are used in place of odorant selective receptor neurons in biological nose, and a pattern recognition system takes place of the signal processing operations in olfactory bulb and brain [7, 8]. The SAW sensors are electronic feedback oscillators whose frequencies change in response to vapor exposure. To achieve this, a SAW device coated with chemically selective polymer thin film is used to control the frequency of oscillations in such a way that selective sorption of vapor molecules in the film generates changes in frequency of oscillation [9, 10]. To make a sensor array for electronic nose, a number of such oscillators are functionalized with different polymer films that respond with varied selectivities towards different chemical species in vapor. On exposure to an odor sample, the sensor array generates a response pattern embedded with odor identity information. The pattern recognition methods extract this information in the form of mathematical descriptors of odor identities (called odor print or signature) for identification [11, 12].

The sensor array based vapor recognition systems rely on the diversity in chemical selectivities of different polymer coatings. The steady state outputs from the array sensors are in proportion to the equilibrium partitioning of vapor molecules into polymer coatings. The partition coefficient defined as the ratio $K = C_p / C_v$, where C_p and C_v denote equilibrium concentration of vapor species in polymer and vapor phases respectively, varies across the array sensors, and is responsible for generating vapor specific response patterns. An alternate approach exploits transient characteristics of sensors output for construction of vapors signature [13-15]. In this approach, only a single sensor is thought to be adequate, as the sensor transients carry information not only about partition coefficients of various chemicals but also about their diffusion kinetics. Different class of vapors therefore produce variations in shapes of transient signals, which may yield vapor signature with proper analysis. Often, wavelet decomposition is used for shape analysis, and the wavelet approximation coefficients, either directly or after some further processing, are taken to represent vapor identities. Most commonly, principal component analysis (PCA) is used post wavelet expansion, where the wavelet approximation coefficients are linearly combined to generate new set of uncorrelated features according to maximum variances [16, 17].

In a recent study [18], the authors proposed a new design and transient analysis approach for the SAW sensor array by using only a single polymer material for coatings. The variability in transients' shapes comes from variations in films thicknesses, because the sensors with different thicknesses reach different stages of equilibration process for a preset vapor sorption-desorption (or sense and purge) time cycle. In this study, we present an information fusion approach based on transient response analysis of SAW sensor array. The method makes use of the wavelet decomposition for information extraction from individual sensors, and then combines the sensor array data for feature extraction by principal component analysis. In the following, we demonstrate that the present approach yields an efficient method for generating high intra-class compaction and inter-class separation for vapor identification. For validation, we employed synthetic data generated by 7-element SAW sensor array which is coated with different thicknesses of polyisobutylene (PIB) film and exposed to various concentrations of seven volatile organic compounds (VOCs), the details of which are presented in the Section 2 below. The data analysis procedure is outlined Section 3, which is then followed by results and discussion in Section 4 and conclusion in Section 5.

2. Data Generation and Wavelet Decomposition

The theory of transient signal generation by a polymer coated SAW sensor under exposure to a vapor sample is described in detail in [18]. It is based on a well-established SAW sensor model [19, 20] and

the theory of in- and out diffusion of vapors in thin polymer films [21]. The details of the single-polymer based multiple-thickness sensor array design (referred to as SPM sensor array) and that of the discrete wavelet decomposition are also described in [18]. The wavelet decomposition of each sensor transient generates a set of wavelet approximation coefficients $[cA_j, j = 1, 2, \dots, N']$ with N' being the number of wavelet coefficients. The latter depends on the number of discrete time points in the transient and the level of wavelet decomposition. The wavelet coefficients can be interpreted as feature components generated by each sensor. Let M denote the number of sensors in the array. Thus, M feature vectors of N' dimensions represent each vapor sample. Because, by design we have applied the same polymer coating material on all the sensors the vapor partition coefficient and diffusion coefficient is common to all the sensors. The difference in feature components is therefore expected to arise from the variations in diffusion profiles because of different stages of termination of equilibration process due to thickness variation. By combining these feature components in some way one may expect to create a better vapor representation.

With this consideration in view, we present an analysis by combining all the feature components from individual M sensors and defining a $N = MN'$ dimensional feature vector representation for a vapor sample. Thus, the data matrix corresponding to P measurements becomes a $P \times N$ matrix, where each the vapor samples are represented along the rows. The columns correspond to wavelet coefficients. The next level of feature generation is then implemented by principal component analysis (PCA). The PCA processing not only reduces dimensionality but also effects fusion of the feature vectors generated by individual sensors of the array. This is so because the principal components are linear combination of primary feature components. In effect, the proposed procedure generates fusion of feature spaces associated with individual sensors to yields new set of decorrelated features. It may be recalled that implementing PCA algorithm seeks decorrelated transformed space.

The details of sensor array design, data generation procedure and wavelet decomposition method are described in [18]. In order that the synthetic data mimics real practical situations, we included an additive noise source in the sensor array outputs. The specifics of SAW sensor array transient response calculations used in the present analysis are described below.

2.1. SAW Sensor Array

Polymer: Polyisobutylene (PIB) having material constants,

Mass density $\rho_p = 0.918 \text{ g cm}^{-3}$,

Storage shear modulus $G_1 = 1 \times 10^9 \text{ dyne cm}^{-2}$,

Loss shear modulus $G_2 = 5 \times 10^8 \text{ dyne cm}^{-2}$,

Storage bulk modulus $K_1 = 1 \times 10^{10} \text{ dyne cm}^{-2}$,

Loss bulk modulus $K_0 = 0 \text{ dyne cm}^{-2}$.

Sensors: 7 SAW oscillator sensors coated with PIB film thicknesses (in nm) 218, 327, 437, 546, 655, 764, 873 corresponding to across thickness phase variations $\phi_3/\pi \leq 0.4$ (that is, from thin film to below resonance conditions [19]). The nominal frequencies of oscillations are assumed to occur at 100 MHz with SAW delay line on ST-X quartz substrate in the feedback.

2.2. Vapor Samples

Vapors: 7 volatile organic compounds (VOCs) with partition coefficient (K) and diffusion coefficient (D) in PIB over 298-325 K are ($K, D \times 10^{-11} \text{ cm}^2 \text{ s}^{-1}$):

Chloroform (200, 260)
 Chlorobenzene (4680, 230)
 o-Dichlorobenzene (22500, 5.49)
 n-Heptane (1200, 48)
 Toluene (1000, 35)
 n-Hexane (180, 160)
 n-Octane (955, 38).

Samples: 10 samples from each vapor class with concentrations varied in the step of 10 ppm over 10-100 ppm range.

2.3. Noise Source

A uniformly distributed additive noise source equivalent to SAW velocity fluctuation over $[-6.3, 6.3]$ ms^{-1} is assumed. This produces SAW oscillators frequency fluctuation over $[-2, 2]$ kHz according to $\Delta v / v_0 = \Delta f / f_0$ where v_0 and f_0 are unperturbed (bare surface) SAW velocity and oscillator frequency respectively.

2.4. Transient Data

Each sensor output record consists of 701 points for 60 sec duration divided into 20 sec sorption and 40 sec desorption intervals. Thus, the 70-samples 7-sensor array transient data is a 3-dimensional matrix of size $70 \times 701 \times 7$. The sensor out is defined as fractional change in frequency with respect to the change produced by polymer coating. That is, the signal

$$s(t) = \left(\frac{\Delta f}{f_0} \right)_{\text{after vapor sorption}} - \left(\frac{\Delta f}{f_0} \right)_{\text{after polymer coating}}, \quad (1)$$

A step vapor exposure with analyte concentration c_0 is assumed occur at time $t=0$. The other details are given in [18]. The data matrix for the analysis purpose is normalized with respect to partition coefficient (K), film thickness (h) and vapor concentration (c_0) according to $s(t) \leftarrow s(t) / Kc_0h$.

2.5. Wavelet Decomposition

Each transient record is processed by discrete wavelet decomposition with Daubechies3 (db3) mother wavelet up to 4th level. The wavelet approximation coefficients were retained and coefficients of detail were discarded as they are known carry noisy components. Thus, each row of data matrix now carries 48 wavelet approximation coefficients corresponding to each sensor. The transient data after wavelet decomposition therefore becomes a matrix of size $70 \times 48 \times 7$.

3. Feature Fusion and Class Separability

The set of wavelet coefficients corresponding to individual sensors for a vapor sample were combined in succession to define $48 \times 7 = 336$ component data vector. Thus the data matrix now becomes a 2-dimensional 70×336 matrix for 70 vapor samples. This data matrix is then processed by principal component analysis (PCA) by taking the wavelet coefficients as variables. The resulting principal

scores are to be the fused feature components, and corresponding principal components eigenvalues define their significance. For comparison, the 70×48 data matrices based on wavelet approximation coefficients corresponding to each sensor were also PCA processed and analyzed in the feature space. In the later analysis, 7 separate feature spaces are created corresponding to 7 sensors. The proposed fusion process initially combines all these spaces into 336 dimensional wavelet coefficient space, which after PCA processing yields fused feature space of lower dimensionality.

The separation of samples belonging to different vapor classes and closeness of within-class samples in feature space measure the vapor discrimination ability of the feature extraction method. A quantitative measure of this is defined by the ratio [22]

$$J = \frac{\text{trace}\{S_m\}}{\text{trace}\{S_w\}}, \quad (2)$$

where S_m denotes the covariance matrix of the PC components defined with respect to global mean (that is, the mean of all samples of all classes) and S_w denotes the weighted covariance matrix defined with respect to class-means. These two matrices are calculated as

$$S_m = (x - \mu_0)(x - \mu_0)^T, \quad (3)$$

$$S_w = \sum_{i=1}^C P_i S_i, \quad (4)$$

where $\mu_0 = \sum_{i=1}^C P_i \mu_i$ is the global mean, $S_i = (x - \mu_i)(x - \mu_i)^T$ is the within-class covariance matrix with μ_i being the class mean, C is the number of classes, $P_i \approx n_i / P$ is the class a priori probability with n_i being the number of samples of i -th class and P the total number of samples. This measure is commonly known as ‘class separability’. It is based on the scatter matrices of principal components, and it provides a basis for comparing the goodness of different data processing methods.

4. Results and Discussion

Fig. 1 shows the transient responses of PIB coated SAW oscillator sensor with film thickness 873 nm (highest used in the array) under exposure to 7 vapors at 10 ppm. It can be seen that the fastest diffusing vapor species (chloroform, chlorobenzene, n-hexane) reach near equilibrium during both sorption and desorption phases, whereas the other 4 vapors are at different stages of equilibration. The polymer film thickness for this sensor corresponds to $\phi_3 / \pi = 0.4$, just below the condition of film resonance [19]. Fig. 2 shows similar transient data generated by all 7 sensors of the array. As pointed out in the beginning, different responses can be seen to be at different stages of the vapor-polymer thermodynamic equilibration.

Fig. 3 shows principal component score plots of the data transformed after wavelet decomposition for two sensors of lowest and highest thicknesses and that after fusion of all the seven sensors data. Fig. 3 (a) and (b) correspond to the single sensor transient based analysis, and Fig. 3(c) is that obtained after fusion. It can be readily noticed that the separation between vapor classes is substantially enhanced after fusion. The inset numbers show the value of class separability measure J . It can be noticed that even though the class separability improves with film thickness, the improvement due to fusion is higher by nearly an order of magnitude. Table 1 shows the first 10 principal component eigenvalues

and cumulative variances for these analyses. It is seen that more than 90 % information lies in these components, the fusion process though generates more even distribution of variances among low eigenvalue high order components. It is expected that the first few components should be good enough for most pattern recognition tasks.

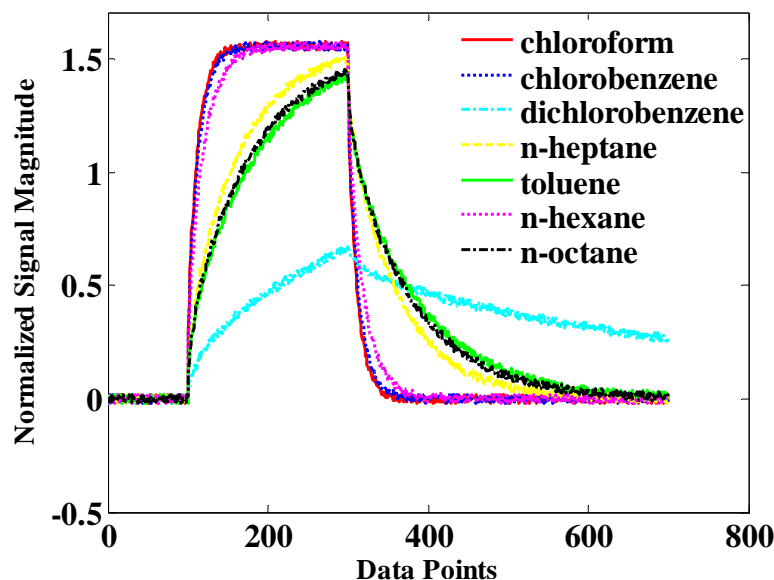


Fig. 1. The normalized transient signals generated by polyisobutylene (PIB) coated SAW oscillator sensor exposed to 10 ppm concentration seven VOCs as indicated. Each data point is separated by 0.1 sec.

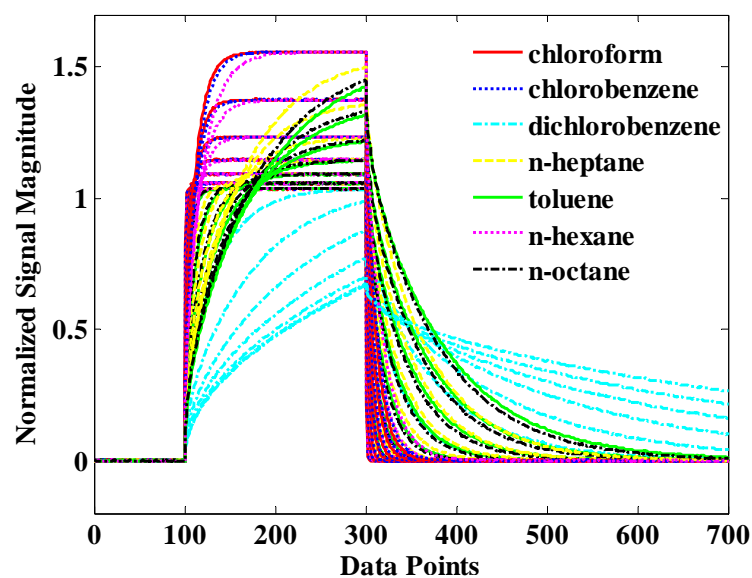


Fig. 2. The normalized transient signals generated by polyisobutylene (PIB) coated multiple (seven) thickness SAW sensor array exposed to 10 ppm concentration of seven VOCs as indicated. Each data point is separated by 0.1 sec.

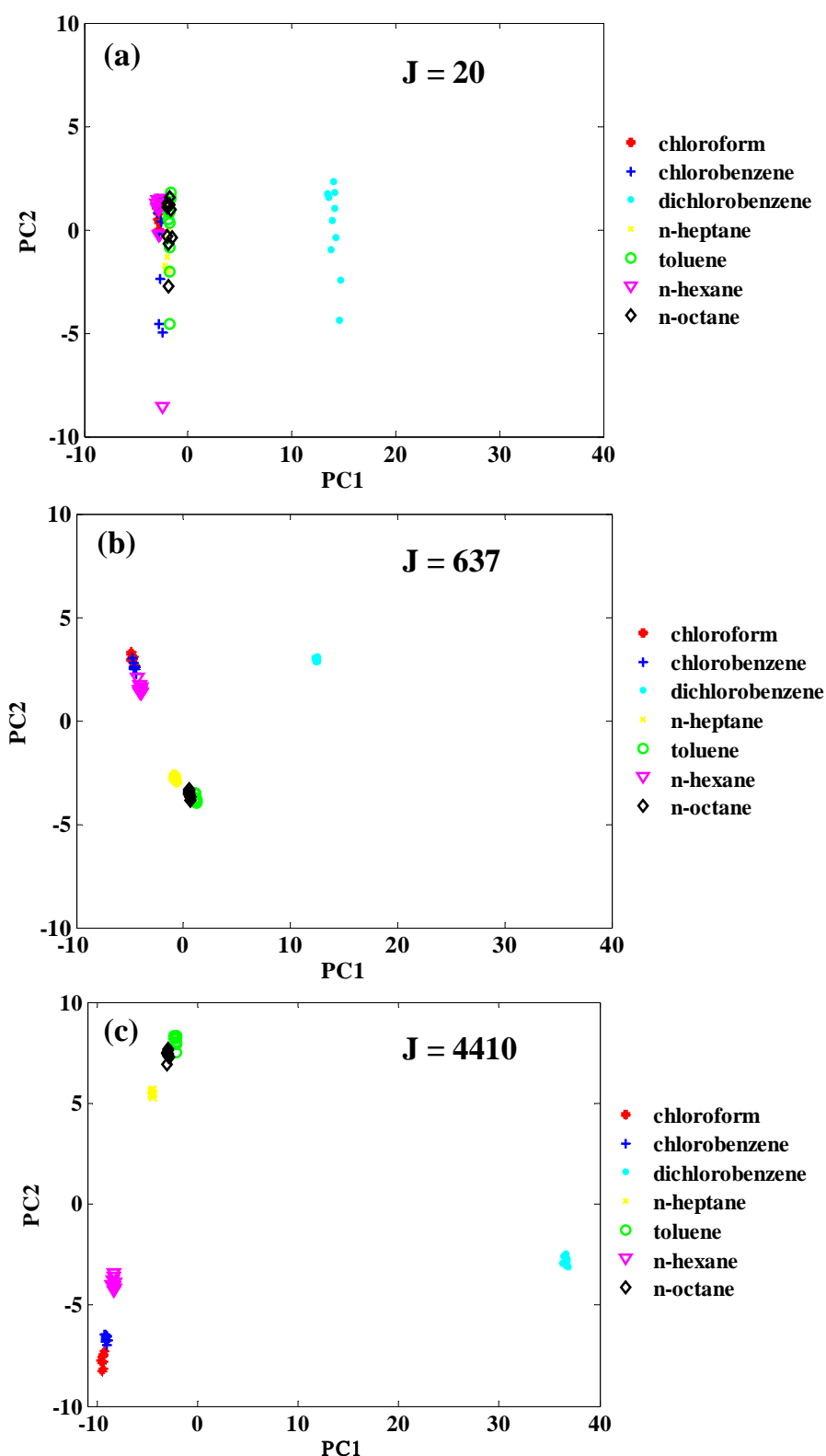


Fig. 3. Principal component score plots using the first two highest eigenvalue components of the transient data transformed by db3 wavelet decomposition to 4th level. (a) based on the single sensor transients having smallest PIB thickness of 218 nm, (b) based on the single sensor transients having largest film thickness of 873 nm, and (c) based on transients of all 7 sensors of the array after fusion. The J-figures shown are the class separability measure.

Table 1. Principal component eigenvalues and cumulative variances of transient data transformed by wavelet decomposition of the two individual sensors with lowest and highest polymer coating thicknesses, and that after fusion of 7-sensor array data.

PC	Sensor 1 (lowest thickness) h = 218 nm		Sensor 7 (highest thickness) h = 873 nm		After fusion of data from all sensors (sensor 1...sensor 7)	
	Eigenvalue	Cumulative variance %	Eigenvalue	Cumulative variance %	Eigenvalue	Cumulative variance %
1	33.61	70.02	31.61	65.87	235.28	70.02
2	3.75	77.85	8.84	84.30	40.47	82.07
3	2.58	83.23	3.54	91.69	5.33	83.65
4	1.31	85.97	1.04	93.87	4.99	85.14
5	1.25	88.58	0.96	95.88	4.79	86.57
6	1.17	91.03	0.89	97.76	3.94	87.78
7	0.96	93.03	0.41	98.62	3.55	88.80
8	0.87	94.87	0.35	99.37	3.03	89.71
9	0.76	96.47	0.22	99.84	2.64	90.49
10	0.55	97.63	0.04	99.93	2.46	91.23

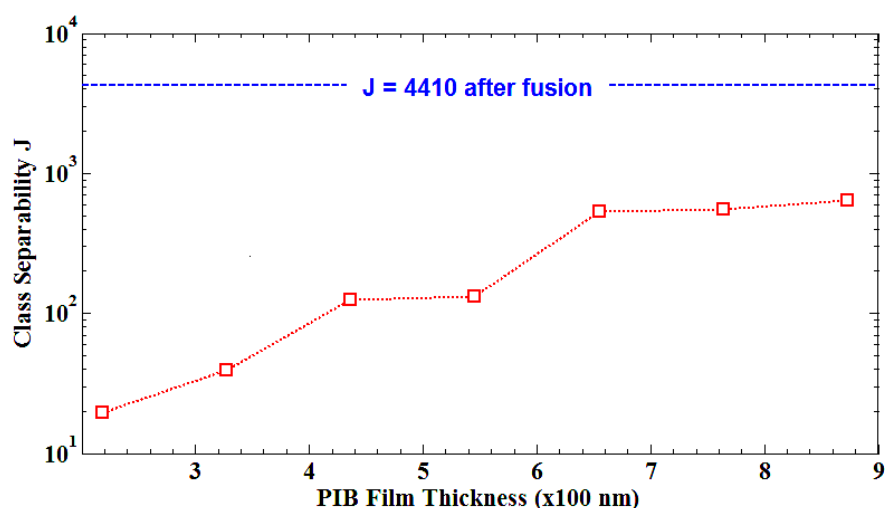


Fig. 4. Variation of class separability J with sensor film thickness h (square marked curve in red). The class separability enhancement achieved after proposed fusion is indicated by the dotted blue line labeled 'J = 4410 after fusion'.

Fig. 4 shows the variation of class separability based on single sensor transients. In addition, indicated in this figure is also the level of class separability reached after sensor array based (wavelet + PCA) based fusion. The proposed fusion method produces separability enhancement by nearly an order of magnitude. Some insight about what produces increased class separability after fusion is obtained by examining the distribution of principal components eigenvalues, Table 1. It is found that beyond first few principal components, the eigenvalues decrease rapidly for single sensor based analyses (see column 2 and 4). In contrast, in the analysis of sensor array based fusion the higher order eigenvalues are more evenly distributed over a large number of components. These high order components beyond the first few (4 or 5) are mainly the noise components. Therefore, by ignoring them the noise components are more effectively eliminated in the fused data analysis. The other important reason lies in the design of variable thickness sensor array itself, which generates information about both the chemical interaction affinities between vapor molecules and polymer and the diffusion kinetics. The wavelet transformed data therefore contains more hidden variables. The PCA combines them linearly

to create an accurate representation of vapor identities. The systematic higher separability achieved by increasing polymer thickness also seems to be due to similar reasons. In thicker films, the nonlinearity in sensor responses due to viscoelasticity might be playing an important role in generating enriched information about vapors.

5. Conclusions

The transient response of single-polymer multiple thickness sensor array when exposed to proper sorption and desorption cycles is laden with information about multiplicity of vapor species chemical interactions with the polymer, and the kinetics of diffusion processes constrained to film boundary conditions. The wavelet transform based shape analysis of transients delineates this information in the form of sets of wavelet coefficients. The principal component analysis of the wavelet coefficients creates vapor identity signatures. The paper examined an information fusion approach for feature extraction by combining the information content inherent in the wavelet coefficients and doing the principal component analysis. The present approach yields nearly an order of magnitude enhancement in the vapor class separability in feature space when compared to single sensor transients.

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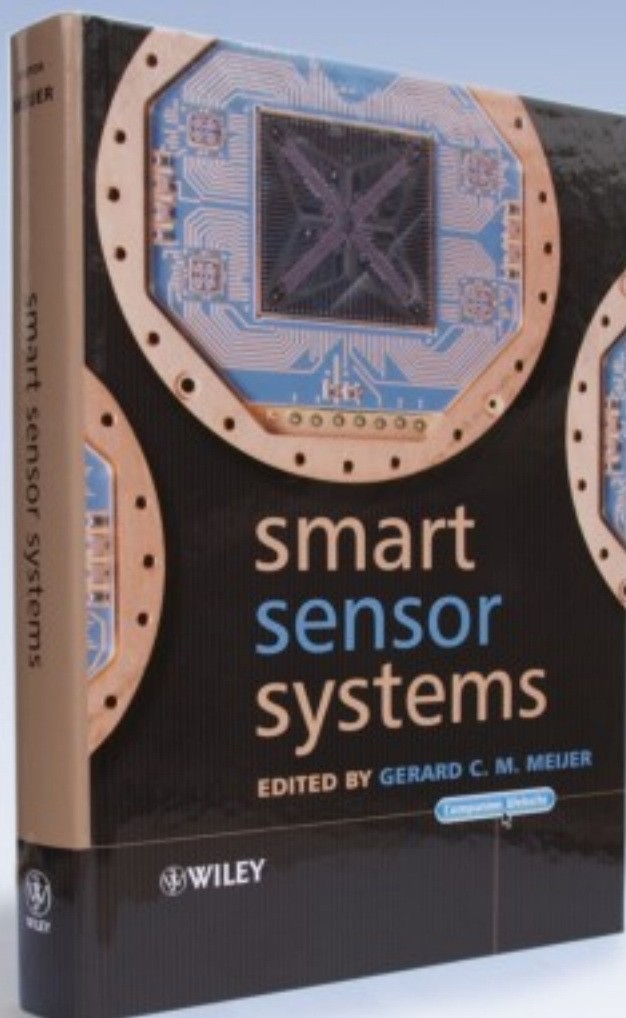
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