A multi-module artificial neural network approach to pattern recognition with optimized nanostructured sensor array

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Abstract

The selection of appropriate sensor array nanomaterials and the pattern recognition of sensing signals are two challenges for the development of sensitive, selective, and cost-effective sensor array systems. To tackle both challenges, the work described in this paper focuses on the development of a new hybrid method which couples multi-module method with artificial neural networks (ANNs) for the optimization—optimized multi-module ANN classifier (OMAC) to enhance the correct detection rate for multiple volatile organic compounds (VOCs). In this OMAC method, each module is dedicated to a group of VOCs with specific inputs. Each sensor element’s selectivity is quantitatively evaluated to assist the selection of sensing array materials, which also facilitates the selection of inputs to each dedicated neural network module. This OMAC method is shown to be useful for achieving a high overall recognition rate for a selected set of vapor analytes. The results are discussed, along with the implications to the better design of ANN pattern classifiers in chemical sensor applications.

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1. Introduction

The large surface area-to-volume ratio, size controllability, chemical stability, and surface tunability of metal or oxide nanoparticles provide an ideal platform for exploring sensing array applications [1]. Indeed, new or improved electronic and optical properties of nanoparticle-structured materials have recently attracted increasing interest in areas of chemical or biological sensors [2–8]. To develop sensitive, selective, and cost-effective sensor array systems, the selection of appropriate sensing array nanomaterials and the pattern recognition of sensing signals are two important challenges. The work described in this paper focuses on the development of a hybrid method to enhance the correct detection rate for different volatile organic compounds (VOCs).

An array of chemiresistive sensors in which each sensor surface is coated with a different nanostructure has recently been demonstrated for detection of VOCs. Since each sensor element may respond to VOCs differently, the responses of a sensor array to a certain VOC will show its unique profile or pattern, which can be utilized for identification of the vapors. Hence, the construction of sensor array system involves the rational selection of the sensing nanomaterials and the pattern recognition of sensing signals, which play important roles in sensor development for accurately detecting the targeted analytes.

Sensing nanomaterials selection is actually a feature space optimization problem for the pattern recognition process, in which the optimal sensors are chosen so that the feature space from the sensor responses for different analytes can be well separated. The pattern recognition in sensor array is a process to detect sample analytes by recognizing certain patterns in the feature space of the sensor array response signals. Although many pattern recognition approaches have been developed, such as statistics method, neural networks, and fuzzy inference systems [9–14], little attention has been given to the optimization of the inputs to pattern classifiers. This paper addresses this...
problem by developing a new hybrid method which couples multi-module method with artificial neural networks (ANNs) for the optimization—optimized multi-module ANN classifier (OMAC). This method is developed to target sensor arrays for detecting multiple VOCs. Based on our previous success in applying ANNs to the nanostructured sensor arrays for the detection of multiple VOCs [15], OMAC method is a more effective multi-module ANNs approach, hybridized with sensor array optimization technology, to pattern recognition for nanostructured array sensing. In this approach, each ANN module is dedicated to a subgroup/class of VOCs. More importantly, each ANN module has its own optimum inputs. This paper describes the results of our study by highlighting the following important aspects: (1) a systematic approach for optimum selection of sensor nanomaterials, (2) pattern recognition techniques using multi-module ANNs, supported by cluster analysis (CA), and (3) input optimization of the sensor responses to each dedicated ANN module.

The following sections discuss the details of the OMAC technology for the construction of nanosensor array systems. Section 2 describes the experiment for sensor array measurements. Section 3 addresses the optimum selection of the sensor coating materials, the construction of an OMAC with optimum inputs, and the comparison of results between OMAC and other methods. Finally, conclusions are drawn in Section 4.

2. Experiment

Details for the preparation of molecularly linked nanoparticle thin film assembly was reported recently [4,15]. The assembly of Au nanoparticles (1.9 ± 0.7 nm, Au nm) by different linkers leads to five types of thin films on interdigitated Pt microelectrodes (IME) devices with interdigitated Pt microelectrodes: (1) NDT-linked nanoparticles (NDT-Au nm), (2) PDT-linked nanoparticles (PDT-Au nm), (3) MUA-linked nanoparticles (MUA-Au nm), (4) MHA-linked nanoparticles (MHA-Au nm), and (5) MPA-linked nanoparticles (MPA-Au nm). (Abbreviations: 11-mercaptoundecanoic acid (MUA), 16-mercaptohexadecanoic acid (MHA), 1,9-nonanedithiol (NDT), and 1,5-pentadithiol (PDT)). The NDT-Au nm coated sensor is denoted as NDT-Au nm/IME. Similar notations are for other coatings, such as PDT-Au nm/IME, MUA-Au nm/IME, MHA-Au nm/IME, and MPA-Au nm/IME.

The sensor measurements have been described in detail in our previous reports [19]. Sensor response measurements were performed using a customized IME device, which has 300 pairs of platinum electrodes of 5 μm width and 5 μm spacing on glass substrate (100 mm thick). The thickness of the coating was below or close to the finger thickness. A computer-interfaced multichannel electrical multimeter (Keithley 2700) was used to measure the partial resistance of the nanostructured coating on IME. The resistance and frequency measurements were performed simultaneously with computer control. All experiments were performed at room temperature, 22 ± 1°C, N2 gas (99.99%, Praxair) was used as reference gas and as diluent to change vapor concentration by controlling mixing ratio. The gas flow was controlled by a calibrated Alaborg mass-flow controller, and the vapor stream was produced by bubbling dry N2 gas through a bubbler of the vapor solvent using the controller to manipulate vapor concentration. Vapors were generated from hexane (Hx, 99.9%, Fisher), benzene (Bz, 99.0%, Fisher), toluene (TL, 99.9%, J.T. Baker), nitrobenzene (NB, 99.9%, Aldrich), p-xylene (p-Xyl, <99%, Aldrich), o-xylene (o-Xyl, 98%, Aldrich), and m-xylene (m-Xyl, ≤99%, Aldrich). The initial ppm concentration (molar (M) or volume (V) concentrations) was calculated from the partial vapor pressure and the gas mixing ratio. The concentrations were given either in ppm (M) or in ppm (V) (= ppm (M)/24.5).

The measured resistance (R) values were expressed as relative differential resistance change ΔRR, for the evaluation of the vapor sorption responses. ΔR is the difference of the maximum and minimum values in the resistance response and R is the initial resistance of the film [4].

3. OMAC method and test results

The selectivity of sensors can significantly influence the correct detection rate of VOCs for a sensor array system. If the sensor films are appropriately selected, selectivity can be notably enhanced by minimizing the similarity of sensor responses to different VOC analytes. It is reported that the performance of a sensor array may degrade when the number of sensors increases beyond a certain number, because of the potential redundant information caused by multiple sensor elements [16–20]. There are some research reports on sensor array optimization using statistical methods and artificial intelligent techniques [21–27]. Different from these methods, first, optimization in OMAC implies two facets: (1) optimum selection of the sensor films for a sensor array as a whole and (2) optimum selection of the sensor responses as inputs to each dedicated ANNs classifiers. Second, our optimization approach is to use the property of multiple concentration levels instead of a single concentration level to rank the selectivity of sensors for different analytes, based on a measure of the response difference among the sensors. The optimum selection of sensors is based on the quantitative evaluation of each individual sensor film, which is described in the following section.

3.1. Selectivity: quantitative analysis

The performance of an individual sensor element is commonly evaluated with four figures of merit: (1) selectivity; (2) sensitivity; (3) response speed; and (4) detection limit. The sensitivity, response speed and detection limit are often used as criteria for initial assessment of an array of sensor films, and they are set to be larger than pre-required threshold values. Under such constrain, the multi-response optimization problem is converted to a single response one.

The selectivity of a film is defined as its capability to identify a test analyte in the presence of other analytes. As one approach to the assessment of the selectivity, it is measured with the ‘distance’ from different analyses in terms of two
parameters: sensitivity and the signal from blank. To demonstrate the methodology, a set of test analytes or VOCs is used, including Hx, Bz, Ti, NB, p-Xyl, o-Xyl, and m-Xyl. To identify the seven different analytes, the relative differential resistance change \( \Delta R/R_i \) of each element in the sensor array is first normalized to the baseline resistance.

The measured signal of a sensor to a certain vapor can be defined as \( S = m \times c + \bar{S}_b \), where \( S \) is the steady-state sensor response signal (i.e., \( \Delta R/\Delta t \)), \( m \) is the response sensitivity, \( c \) the gas mixing ratio of the vapor flow versus the total flow of vapor and nitrogen, and \( \bar{S}_b \) is the signal from blank. The conversion between the ppm concentration (ppm (M)) and the gas mixing ratio \( c \) (%) is shown in Table 1.

Fig. 1 shows a set of the response signal \( S \) versus gas mixing ratio \( c \) (%) for five different sensor array materials, in response to the seven different vapors at 10 different concentration levels. Theoretically, the signal \( S \) of a vapor can be distinguished from other vapors if either the value of its sensitivity \( m \ug{\Delta R/\Delta t} \) or the signal from blank \( \bar{S}_b \) is different from others. Thus, these two variables are used to represent the separation capability of each sensor element for different vapors. Fig. 2a–e visually demonstrates

![Graphs and diagrams]

**Table 1**

<table>
<thead>
<tr>
<th>Concentration (%)</th>
<th>Hx</th>
<th>Bz</th>
<th>Ti</th>
<th>NB</th>
<th>p-Xyl</th>
<th>o-Xyl</th>
<th>m-Xyl</th>
</tr>
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<tbody>
<tr>
<td>5</td>
<td>413</td>
<td>259</td>
<td>78</td>
<td>0.7</td>
<td>24</td>
<td>18</td>
<td>18</td>
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<tr>
<td>10</td>
<td>825</td>
<td>519</td>
<td>155</td>
<td>1.4</td>
<td>48</td>
<td>36</td>
<td>36</td>
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<tr>
<td>15</td>
<td>1238</td>
<td>778</td>
<td>233</td>
<td>2.1</td>
<td>72</td>
<td>54</td>
<td>54</td>
</tr>
<tr>
<td>20</td>
<td>1651</td>
<td>1037</td>
<td>310</td>
<td>2.8</td>
<td>95</td>
<td>72</td>
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<td>25</td>
<td>2063</td>
<td>1296</td>
<td>388</td>
<td>3.5</td>
<td>119</td>
<td>90</td>
<td>89</td>
</tr>
<tr>
<td>30</td>
<td>2476</td>
<td>1556</td>
<td>465</td>
<td>4.2</td>
<td>143</td>
<td>108</td>
<td>107</td>
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<tr>
<td>35</td>
<td>2888</td>
<td>1815</td>
<td>543</td>
<td>5.0</td>
<td>167</td>
<td>126</td>
<td>125</td>
</tr>
<tr>
<td>40</td>
<td>3301</td>
<td>2074</td>
<td>621</td>
<td>5.7</td>
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<td>144</td>
<td>143</td>
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<tr>
<td>45</td>
<td>3714</td>
<td>2333</td>
<td>698</td>
<td>6.4</td>
<td>215</td>
<td>163</td>
<td>161</td>
</tr>
<tr>
<td>50</td>
<td>4126</td>
<td>2593</td>
<td>776</td>
<td>7.1</td>
<td>239</td>
<td>181</td>
<td>178</td>
</tr>
</tbody>
</table>

**Fig. 1.** Sensor response signal \( S \) vs. the gas mixing ratio \( c \) (%) for seven vapors with five different sensing array materials: (a) NDT-Aunm, STD: Hx (0.0394), Bz (0.0554), Ti (0.0498), NB (0.0055), p-Xyl (0.0392), o-Xyl (0.0385), m-Xyl (0.0393); (b) PDT-Aunm, STD: Hx (0.0292), Bz (0.0430), Ti (0.0396), NB (0.0083), p-Xyl (0.0287), o-Xyl (0.0277), m-Xyl (0.0287); (c) MUA-Aunm, STD: Hx (0.235), Bz (0.4629), Ti (0.449), NB (0.0542), p-Xyl (0.440), o-Xyl (0.498), m-Xyl (0.443); (d) MHA-Aunm, STD: Hx (0.325), Bz (0.607), Ti (0.585), NB (0.0403), p-Xyl (0.560), o-Xyl (0.597), m-Xyl (0.561); and (e) MPA-Aunm, STD: Hx (0.0121), Bz (0.0227), Ti (0.0213), NB (0.00794), p-Xyl (0.0167), o-Xyl (0.0368), m-Xyl (0.0175). Standard deviations (S.D.) are included in the parentheses. Vapor: Hx (●), Bz (□), Ti (▲), NB (▲), p-Xyl (◇), o-Xyl (■), and m-Xyl (▼).
each sensor’s separation capability for the aforementioned seven vapors. The distance between two VOCs (two points in the figure) represents the response difference of two different VOCs by an individual sensor element, of which a longer distance implies a larger response difference. An individual sensor element shows good selectivity to certain VOC, if the position of this VOC is far away from others in Fig. 2. Generally, higher degree of scattering of data points in Fig. 2 denotes higher selectivity of the corresponding sensor element to the seven test VOCs. It is observed that data points are significantly scattered in Fig. 2c and d, while not in Fig. 2a, b, and e, which means that MUA-Aunm and MHA-Aunm have better selectivity for the seven vapors than the other three films. Particularly, all the points are almost overlapped in Fig. 2e, which implies that MPA-Aunm has the lowest selectivity.

To quantify the above qualitative description of the selectivity, a new term ‘separation distance’ defined as the Euclidean distance between every two points in Fig. 2 is further introduced. The separation distance between two different test vapors on kth sensor element is given in Eq. (1).

$$d_{ij}(k) = \sqrt{(s(i, k) - s(j, k))^2 + (\bar{S}_{bl}(i, k) - \bar{S}_{bl}(j, k))^2},$$

where $d_{ij}$ is the distance between the i\textsuperscript{th} and j\textsuperscript{th} vapors on the k\textsuperscript{th} sensor element, $s(i, k)$ and $\bar{S}_{bl}(i, k)$ the sensitivity and the signal from blank, respectively, for the i\textsuperscript{th} vapor on the k\textsuperscript{th} sensor element, and $m$ and $n$ are the number of the sensor elements and test vapors, respectively.
different sensor films may be good at separating different vapors, separation distance for each vapor-film pair varies greatly. While five sensor films is summarized in Fig. 3. It is observed that the can be better separated by sensor films NDT-Aunm, PDT-Aunm, different vapor, whereas Fig. 3 summarized the minimum separation distance for the seven vapors on the five sensor films. The different measures needed. We consider the following several different measures based on the film’s minimum separation distance \(d_{ij}(k)\) to each vapor: the film’s minimum separation distance denotes how well the two closest samples can be distinguished. The average separation distance denotes the film’s average separation capability for a set of test vapors. The maximum separation distance denotes the highest separation capability that the film has for a set of VOCs. Generally, a film can be considered to have good selectivity when \(D_{\text{max}}(k)\), \(D(k)\), and \(D_{\text{ave}}(k)\) display values which are sufficiently large. The value of these three measures for the five films is summarized in Table 2.

![Fig. 3](image)

The minimum separation distance for different VOCs on the different sensor films.

The selectivity of a film to a vapor can be measured with the minimum separation distance of the i-th test vapor on the k-th sensor element, \(d_{ij}(k)\), of which is given by Eq. (2). A larger value for the minimum separation distance means that the film has better capability to distinguish one vapor from the other vapors.

\[
d_{ij}(k) = \min_{j:1,2,\ldots,n} \{d_{ij}(k)\}, \quad i = 1,2,\ldots,n; \quad k = 1,2,\ldots,m,
\]

where \(i, j\) are the two indexes representing different vapors, \(n\) the total number of test vapors, \(k\) the index representing different films and \(m\) is the total number of films.

The minimum separation distance for the seven vapors on the five sensor films is summarized in Fig. 3. It is observed that the separation distance for each vapor-film pair varies greatly. While different sensor films may be good at separating different vapors, there is not a single film of which is good for distinguishing all the vapors. For example, with NDT-Aunm as sensing film, Hx and NB can be better separated as compared with other VOCs, whereas the separation for p-Xyl is the poorest. Another example is that most of these vapors seem to be well separated with MHA-Aunm except TI and m-Xyl. In summary, signals of Hx and NB can be better separated by sensor films NDT-Aunm, PDT-Aunm, MUA-Aunm, and MHA-Aunm than the film MPA-Aunm. All of the five films have similar separation performance pattern on the three xylenes. NDT-Aunm, PDT-Aunm, and MUA-Aunm showed a relatively small separation distance to Brz and TI, whereas MHA-Aunm has a relatively large separation distance to Brz. Based on the above discussion, the rank for the first three selections of sensors for each film is shown in Fig. 4. It is important to note that Fig. 4 presents the rank of sensors selection for detecting different vapor, whereas Fig. 3 summarized the minimum separation distance for the seven vapors on the five sensor films. The conclusion provides an important base to construct the pattern classifier in the following sections.

Since individual sensors have different separation capabilities to different VOCs, as shown in Figs. 2 and 3, a quantitative evaluation of the overall selectivity of a film to \(n\) test vapors is needed. We consider the following several different measures based on the film’s minimum separation distance \(d_{ij}(k)\) to each vapor: the film’s minimum separation distance \(D_{\text{ave}}(k)\) to \(n\) test vapor, the average separation distance \(\bar{D}(k)\) to each test vapor, and the maximum separation distance \(D_{\text{max}}(k)\) to each test vapor. These three measures are given by Eqs. (3)–(5), respectively. The film’s minimum separation distance denotes how well the two closest samples can be distinguished. The average separation distance denotes the film’s average separation capability for a set of test vapors. The maximum separation distance denotes the highest separation capability that the film has for a set of VOCs. Generally, a film can be considered to have good selectivity when \(D_{\text{ave}}(k)\), \(\bar{D}(k)\), and \(D_{\text{max}}(k)\) display values which are sufficiently large. The value of these three measures for the five films is summarized in Table 2.

\[
D_{\text{ave}}(k) = \frac{1}{n} \sum_{i=1}^{n} d_{ij}(k), \quad i = 1,2,\ldots,n; \quad k = 1,2,\ldots,m,
\]

(3)

\[
\bar{D}(k) = \frac{1}{n} \sum_{i=1}^{n} d_{ij}(k),
\]

(4)

\[
D_{\text{max}}(k) = \max_{i=1,2,\ldots,n} d_{ij}(k),
\]

(5)

where \(i, j, n, k\) are the same index with Eq. (2).

To compare the separation capability of sensors, a term “relative selectivity” is introduced here, which is defined as the logarithm combination of the ranks of each film under each one of the above three measures, as given in Eq. (6).

\[
r(k) = \frac{1}{m} \sum_{i=1}^{m} w_{i,k} \log (\frac{1}{r_{i,k}}), \quad k = 1,2,\ldots,m.
\]

(6)

where \(l\) is the number of measures, \(r_{i,k}\) the rank of the film \(k\) under measure \(l\), and \(w_{i,k}\) is the pre-selected weight for the \(l\)th measure of the \(k\)th film.

The relative selectivity data are compared and summarized in Table 3. A smaller value of \(r(k)\) indicates the achievement of a better selectivity for all seven vapors. It is observed that MHA-Aunm has the highest relative selectivity for the test VOCs, whereas MPA-Aunm displays the poorest one. If a threshold is set to 2.0 for the relative selectivity \(r\), MPA-Aunm can be eliminated from the original sensor array.

![Table 3](image)

The rank of the relative selectivity for the five sensors to the seven test VOCs.
Fig. 4. The rank of sensors selection for each vapor.

It is interesting to observe that the overall selectivity rank displays a linear trend for the five sensing nanomaterials. While the exact origin of the linearity is part of our on-going research, we believe that this trend partially reflects the trend of the interparticle spatial properties of these nanostructures. In terms of interparticle spacing defined by the linker molecule, the rank of the five nanostuctured films is: MPA-Anm < PDT-Anm < NDT-Anm < MUA-Anm < MHA-Anm. Another important factor involves the difference of functional groups among these nanostructures, which is partially responsible for the difference in sensor selectivity.

Having discussed about the selection of the sensor elements, the following subsections focus on the discussions on how to construct multi-module ANNs classifier for sensor array data processing and vapor recognition.

3.2. Pattern recognition with BP-based multi-module classifier

There are many existing approaches to pattern recognition with sensor arrays, including, artificial neural networks (ANNs) [2], cluster analysis (CA) [3], and principal component analysis (PCA) [4] techniques. Among all these methods, ANNs are universally recognized as one of the most effective approaches. However, the current ANNs applications in sensor array only involve single ANN module/architecture, which is very difficult to simultaneously obtain the satisfying correct identification rates for multiple VOCs. This paper addresses a more sophisticated multi-module ANNs approach with each module dedicated to a sub group/class of VOCs. This paper addresses the results of sensor optimization for each vapor subgroup. The CA technique is discussed in the next subsection for arranging the vapors to different groups, with each group having a dedicated intelligent classifier, before individual vapor is identified. The objective of this step is to further enhance the correct recognition rate for each individual vapor. The grouping task is accomplished by cluster analysis technique with K-clustering algorithm.

CA is a statistical method for assigning sets of similar items into different groups (clusters) with meaningful structures. There are different algorithms and approaches for clustering [28]. The K-clustering algorithm is one of the most common nonparametric partition-clustering one for exclusive test patterns which attempts to find a K-clustering with minimal MSE [28]. In other words, its goal is to minimize dissimilarity in the items within each cluster while maximizing the value between items in different clusters. It searches for the best set of clusters centroids, and determines the structure of the partition by assigning each input vector to its nearest centroid. The centroid of a cluster is defined as the point whose value are the average values of every point in the current cluster. The distance to the centroids is calculated based on Euclidean distance metric, which is given by Eq. (7) [28]:

$$Ed_{ij} = \sqrt{\sum_{k=1}^{n}(x_{ik} - x_{jk})^2}, \quad (7)$$

where $Ed_{ij}$ is the Euclidean distance between patterns $x_i$ and $x_j$, each with $n$ samples.

In this study, CA method is applied to cluster the seven tested vapors into a couple of groups based on their Euclidean distance. The similarity level ($S_{ij}$) between two individual data sets is evaluated based on the distance [29]:

$$S_{ij} = \frac{100(1 - Ed_{ij})}{\text{Max}(Ed_{ij})}. \quad (8)$$
The similarity levels are then used to group the vapors into subgroups. The members in the same group share certain properties in common. The cluster analysis result for the seven vapors is shown in Fig. 5. It is implied that the seven vapors could be clustered into two basic groups with group I (red color in Fig. 5) consisting of Hx and NB, and group II (green color in Fig. 5) consisting of Bz, TL, p-Xyl, o-Xyl, and m-Xyl. Group II can be further classified into two subgroups, one containing Bz, TL, and the other consisting of p-Xyl, o-Xyl, and m-Xyl.

In the next subsection, multiple dedicated artificial neural networks are employed to recognize each individual vapor.

3.2.2. Artificial neural network classifier

Based on the above cluster analysis result, an intelligent classifier with multi-module (or multi-level) neural network is constructed with each one dedicated to specific vapor group to perform vapor recognition. Each module consists of a back propagation network (BPN) with its own suitable architecture. The advantage of the multi-module ANNs is to eliminate the need for accommodating all the identification knowledge, weights stored in the ANNs, for all target vapors in a single network. By using multiple networks, each network is trained for learning more specific knowledge on certain vapors. In this way, the overall correct recognition rate is enhanced by "multiple experts".

To classify the aforementioned seven test VOCs, a two-level BPN-based classifier system is constructed, as shown in Fig. 6a. There are one cluster engine in the first level of the classifier system and three vapor recognizers in the second level. The cluster engine and vapor recognizers are constructed with four different BPNs, respectively. The process of vapor detection is summarized in Fig. 6b. After preprocessed, the sensor array response signals are first classified into one of the two groups with the cluster engine (Group I: Hx and NB; Group II: Bz, TL, p-Xyl, o-Xyl, and m-Xyl). Then, the vapors belong to group I are classified with the vapor recognizer I (BPN1) of the second level networks I. The others are classified into one of the three categories with vapor recognizer II (BPN2): Bz, TL, and Xyl. If the output of recognizer II is Xyl, recognizer III (BPN3) is applied to further identify which of the following classes it belongs to: p-Xyl, o-Xyl, or m-Xyl.

3.3. Evaluation of the method

For comparison purpose, two multi-module ANNs-based intelligent classifiers are developed: one with the optimized sensor array and also optimized inputs to each ANN module, and the other with the original sensor array and all signals serve as the inputs to each ANN module. Different BPN net architectures have been explored and the ones resulted in best recognition rate have been selected for each classifier.
The classifier with the optimized sensor array analysis signals come from four sensors (NDT-Aunm, PDT-Aunm, MUA-Aunm, and MHA-Aunm) instead of original five sensors, in which MPA-Aunm is eliminated. The seven vapors are first assigned into three groups according to their similarity by cluster engine (as mentioned in Section 3.1, and served as inputs to three corresponding ANNs). Each group was further selected based on their selectivity mentioned in Section 3.1, and served as inputs to three corresponding vapor recognizers (three BPNs with architecture 4 × 4 × 2, respectively) to perform classification, as shown in Fig. 7a. The first two ANNs use all four sensor responses for the classification, while the third ANN only uses two sensor responses: MUA-Aunm and MHA-Aunm.

The multi-module classifier without sensor optimization which uses all the five sensor array responses for every group and all feeds into each BPN, was also constructed for classifying the same vapors, as shown in Fig. 7b. The structures of these two different sensor systems are compared in the following paragraphs.

In the data analysis, a total of 140 sets of data were collected from which 75% were used as training data sets and 25% were used as verifying data sets. Twenty sets of testing patterns were also obtained for each vapor at 10 different concentration levels. In this study, instead of using threshold limits, the analyte is defined as present if the value of the corresponding output is the maximum among all of the outputs, or absent if the value of the output is smaller than anyone of the others. The recognition rates of both classifiers are summarized in Table 4.

Table 4
The recognition rate of classifiers with and without optimizing sensor array

<table>
<thead>
<tr>
<th>Sensor array optimization</th>
<th>Hx</th>
<th>Br</th>
<th>Ti</th>
<th>NB</th>
<th>p-Xyl</th>
<th>o-Xyl</th>
<th>m-Xyl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optimized (see Fig. 7a)</td>
<td>100</td>
<td>100</td>
<td>90</td>
<td>100</td>
<td>100</td>
<td>80</td>
<td>80</td>
</tr>
<tr>
<td>Not optimized (see Fig. 7b)</td>
<td>90</td>
<td>100</td>
<td>90</td>
<td>100</td>
<td>40</td>
<td>90</td>
<td>40</td>
</tr>
</tbody>
</table>

All values are in percentage.

It is observed that the classifier with optimized sensor array has significantly higher classification capability than the other one, especially for xylene classification. Its overall recognition rate for all vapors is satisfactory in spite of the fact that the recognition rate of m-Xyl is a little lower than other vapors. For the classifier without optimizing sensor array and inputs to each ANN, the recognition rates for p-Xyl and m-Xyl are both lower than 50%. From the comparison, it is clearly demonstrated that our OMAC method described in this paper is very effective in enhancing the correct vapor identification rate.

4. Conclusion

In conclusion, we have developed an OMAC method which couples multi-module method with ANNs for the optimization to enhance the correct detection rate for multiple VOCs using nanostructured sensing arrays. The selection of sensor elements and the construction of ANN pattern classifier are shown to be important components for improving the performance of the nanostructured sensor array system. Some of the most significant aspects of our approach involve the selection of sensor elements, construction of multi-module ANNs, and selection of the inputs to each ANN. The results from processing the experimental data have demonstrated the effectiveness of our hybrid method in enhancing the overall recognition rate for the detection of multiple VOCs. In addition, the cluster analysis is proven to be an effective way to support the construction of the multi-level ANNs.

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References


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