Steady-state response feature extraction optimization to enhance electronic nose performance

Dyah Kurniawati Agustika
School of Engineering
The University of Warwick
Coventry, United Kingdom
Dept. of Physics Education
Universitas Negeri Yogyakarta
Sleman, Indonesia
Dyah.Agustika@warwick.ac.uk

Shidiq Nur Hidayat
Physics Department
Universitas Gadjah Mada
Sleman, Indonesia
shidiq.nurhidayat@mail.ugm.ac.id

Kuwat Triyana
Physics Department
Universitas Gadjah Mada
Sleman, Indonesia
triyana@ugm.ac.id

Doina Daciana Iliescu
School of Engineering
The University of Warwick
Coventry, United Kingdom
D.D.Iliescu@warwick.ac.uk

Mark Stephen Leeson
School of Engineering
The University of Warwick
Coventry, United Kingdom
Mark.Leeson@warwick.ac.uk

***Abstract*—Feature extraction of electronic nose (e-nose) output response aims to reduce information redundancy so that the e-nose performance can be improved. The use of different sensor types and sample targets can affect the optimization of feature extraction. This research used six types of metal oxide sensors, TGS 813, 822, 825, 826, 2620, and 2611 in an e-nose system to detect three types of herbal drink. Five kinds of feature extraction methods on the original response curve in a steady-state response were used, namely, baseline difference, logarithmic difference, local normalization, global normalization, and global autoscaling. The results of feature extraction were fed into a Principal Component Analysis (PCA) system. As a result, global autoscaling and normalization had the highest total sum of the first and second principal components of 96.96%, followed by local normalization (90.18%), logarithm, and baseline difference (88.92% and 79.26%, respectively). The validation of PCA results was performed using a Backpropagation Neural Network (BPNN). The highest accuracy, 97.44%, was obtained from the global autoscaling method, followed by global normalization, local normalization, logarithm, and baseline difference, with an accuracy level of 94.87%, 92.31%, 89.74%, and 82.05%, respectively. This demonstrates that the selection of the feature extraction method can affect the classification results and improve e-nose performance.**

Keywords—electronic nose, feature extraction, Principal Component Analysis, Backpropagation Neural Network

I. INTRODUCTION

The selection of the ingredients with high quality and the determination of shelf-life are the main things in the beverage industry. This mainly uses human sensory panels to evaluate the quality of the ingredients [1]. While determining the shelf-life is usually carried out by storing food products in a certain temperature range, including the highest limit [2]. Nonetheless, these methods have some drawbacks. For human sensory panels, even for trained evaluators, psychological and physical variability can influence judgment, and individual preferences can be biased and susceptible to variations in large odor sources [3]. In addition, humans are unable to smell certain compounds at the highest concentration [1]. Meanwhile, storing beverages under certain temperatures for determining the shelf-life takes considerable time and is costly.

There are sophisticated technologies for the quality assurance of the products, such as Gas-Chromatography [3]. However, small and medium sized enterprises have difficulty accessing such advanced methods [4] that can help them determine the quality of ingredients and shelf life. Therefore, a reliable and inexpensive instrument for quality testing and shelf-life determination for the small and medium sized enterprises is needed.

The electronic nose (e-nose) is a reliable and inexpensive instrument used to test the quality and determine the shelf-life of beverages. Eriksson *et al.* discriminated milk obtained from healthy cows and those suffering from acute clinical mastitis using an e-nose [4]. Gamboa *et al.* determined the wine quality from the presence of acetic acid by using thin-film semiconductors [5]. Tudu *et al.* distinguished the quality of five different black teas by using an e-nose based on the leaf quality, inspection, and combined perception of aroma and flavour [6]. Hidayat *et al.* used eight metal oxide semiconductors to classify the quality grades of java cocoa beans [7], and Labreche *et al.* determined the shelf-life of milk using an e-nose [8].

An e-nose is used to detect volatile and odor compounds. It consists of sensor array units, signal conditioning systems, pre-processing systems, and pattern recognition algorithms [9], [10]. E-noses can provide fast, automatic, and real-time classification and detection [4], [9]. Moreover, they can easily be retrained to fit different applications to detect various odors. However, the difficulty in achieving reproducibility and sensor selectivity results in diminishing e-nose performance. As a consequence, the use of e-noses in the industrial world to date has been modest [11].

The limitations of an e-nose can be addressed by sensor array optimization and specific sensor selection. Nevertheless, this only applies to a bespoke e-nose, whereas for a commercial one, the hardware structure cannot be changed. In addition to these methods, optimization can also be performed by feature extraction and selection of appropriate pattern recognition models [12].

Feature extraction aims to reduce data redundancy by selecting important information from the output response so that the pattern recognition process can run effectively. There are various types of feature extraction. First, feature extraction can be performed on the original response curve at the steady-state or transient response; this method includes extraction of the maximum value, baseline difference, logarithmic difference, local and global normalization, and the area under the sensor output response. The second extraction is based on curve fitting. This is performed by constructing a curve with certain mathematical equations with the best fitting of the signal response, and then the curve parameters are used for extraction. The third extraction is achieved by transforming the signal using methods such as the discrete wavelet transform (DWT) [12].

The feature extraction method has been demonstrated in improving e-nose performance. Hidayat and Triyana applied a baseline difference in the signal response of an e-nose in Tempeh's fermentation process [13]. Meanwhile, Agustika and Triyana used the DWT as a feature extraction method to distinguish herbal drinks [14]. However, both papers did not discuss the reason why such methods were chosen. Therefore, in this paper, the reason behind the selection of several feature extraction methods is explained in Section II. Furthermore, the methods are then optimized to get the best result of classification.

Optimization of the e-nose can also be undertaken by selecting the appropriate pattern recognition system. Several pattern recognition algorithms are applied to improve e-nose performance, such as principal component analysis (PCA), linear discriminant analysis (LDA), discriminant function analysis (DFA), support vector machine (SVM), and artificial neural network (ANN) [15].

In this research, an e-nose is used to distinguish traditional beverage products, namely *Beras Kencur*, *Kunir Asem*, and *Temu Lawak*, which are herbal drinks that can be found in local markets in Indonesia, especially in Java. These drinks are used as traditional herbal medicine that is made mostly by small and medium sized enterprises. The research was performed in a part to apply an e-nose to the products of small and medium sized enterprises. In the future, the producer could also implement the e-nose as a tool to test the quality of their products.

The performance of the e-nose was improved by optimizing the feature extraction. E-nose output signals from the original curve response in a steady-state were processed using five different methods: baseline difference, logarithm difference, local normalization, global normalization, and global autoscaling. Feature extraction results were fed into the PCA pattern recognition system to find the most optimized feature extraction method for discriminating herbal drinks in the e-nose system. Furthermore, for PCA result validation, the Backpropagation algorithm Neural Network was used.

II. Materials and Methods

A. Materials

The materials used in this experiment were kinds of herbal drinks from a traditional market in Yogyakarta, Indonesia, namely, *Beras Kencur*, *Kunir Asem*, and *Temu Lawak*. The first consists of a mix of rice, sugar, and galanga, the second comprises a mixture of turmeric, sugar, and tamarind, and the third contains only Curcuma. The ingredients of each kind of drink are blended with water to make herbal drinks. The concentration of samples was not measured to simulate the real conditions and testing the ability of e-nose to differentiate types of odour without regard to the concentration. Each type of herbal drink was divided into 15 samples with the same volume. The fresh samples were stored in 40 mL vials.

The e-nose used consisted of six metal oxide Taguchi Gas Sensors (TGSs), the specifications of the type of gas sensor and the main target gas are given in TABLE I, while the picture of the array of sensors is given in Fig 1.

TABLE I. Kinds of Gas Sensor and the Targeted gas

Types of Sensor	Target Gasses
TGS813	Methane, Liquefied petroleum gas [16]
TGS822	Organic solvent vapors [17]
TGS825	Hydrogen sulfide [18]
TGS826	Ammonia [19]
TGS2611	Methane [20]
TGS2620	Alcohol and Organic solvent vapors [21]

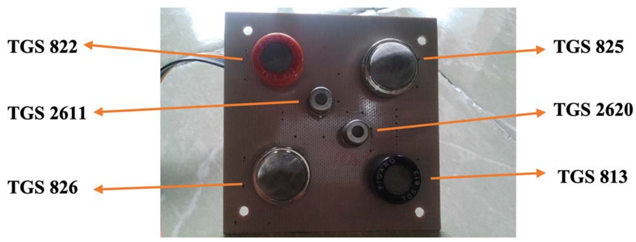

Fig 1. Array of Sensors

B. Methods

The diagram of the e-nose system used in this research is depicted in Fig 2. The sample vial was placed in the sample chamber, which was equipped with a temperature regulator to heat the sample. The system was equipped with two fans. Fan 1 functioned to suck the sample aroma into the array of sensors, and Fan 2 was to clean the sensors. TGS gas sensors in the array of sensors are a type of metal oxide sensor, and if the target gas interacts with the surface layer on the sensor, there will be a change in the sensor resistance [22]. To measure changes in sensor resistance, a voltage divider was used. The voltage divider circuit's output voltage is still an analog form, and this voltage was converted to digital form by a Data Acquisition (DAQ) system [23]. Sensor output responses in digital form were stored by the computer and used for further analysis.

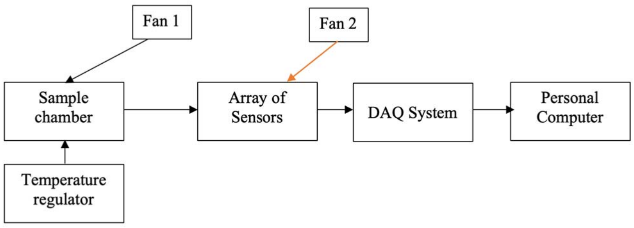

Fig 2. Block diagram of the e-nose used

Prior to data collection, the gas sensor array on the e-nose was heated for 10 minutes to reach the sensor working point, after which the testing process began. Before bringing the sample into the sensor room, Fan 1 was turned on to obtain the baseline value, which is the sensor value when exposed to the ambient air. After that, the sample was put into the sample chamber, and Fan 1 sucked in the sample to be exposed to the sensor room. Fan 1 turned on for 1 minute, with a sampling frequency of 0.2 Hz, so there were 12 data points in 1 minute. After the sampling process, Fan 2 (indicated by the orange arrow) turned on for 120 seconds to clean the sensor chamber. The signal response of TGS 825 in the *Temu Law*ak sample is shown in Fig 3. The image depicts the response of the gas sensor when the sensor is exposed to ambient air (baseline phase), sample exposure (consists of transient and steady-state response), and purging.

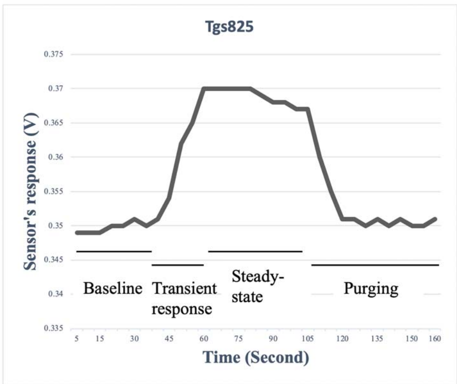

Fig 3. Signal response of TGS 825 for Temu Lawak

The e-nose output response was stored on the computer for further analysis. The first step in the analysis stage was pre-processing, and in this study, feature extraction and data compression were used. Then, the signal response that has been pre-processed, fed into a pattern recognition system, PCA. The results of that were then compared to find the most suitable feature extraction method. It was then validated by using a Backpropagation Neural Network.

III. Results and Discussion

A. Feature Extraction

The data from the steady-state response (see Fig 3) was used for further analysis. Steady-state is often used because it describes the balance of the whole dynamic process that represents the sensor's response to odours [12]. The descriptors were taken to start from the fourth point in the signal response during sample exposure to the twelfth point, right before the purging stage started; hence there are nine data points for one signal response. The data points were then used for feature extraction.

There were five methods of feature extraction on the original curve response used. First, the baseline difference [12], [24],

$$x_{ij}^{(k)} = V_{ij}^{(k)} - V_{ij}^{(ref)} \qquad (1)$$

second, the logarithm difference[12]

$$x_{ij}^{(k)} = \log\left(\frac{V_{ij}^{(k)}}{V_{ij}^{(ref)}}\right) \qquad (2)$$

third, the local normalization [22]

$$x_{ij}^{(k)} = \frac{V_{ij}^{(k)}}{\sqrt{\sum_i V_{ij}^{(k)^2}}} \qquad (3)$$

fourth, the global normalization [22]

$$x_{ij}^{(k)} = \frac{V_{ij}^{(k)} - \min[V_i]}{\max[V_i] - \min[V_i]} \qquad (4)$$

and fifth, the global autoscaling [22]

$$x_{ij}^{(k)} = \frac{V_{ij}^{(k)} - \text{mean}[V_i]}{\text{std}[V_i]} \qquad (5)$$

$x_{ij}^{(k)}$ is the response from the *i*-th sensor to sample *j* that has been feature extracted, $V_{ij}^{(k)}$ is original curve response from the *i*-th sensor to sample *j*, $V_{ij}^{(ref)}$ is the mean value of the baseline from the *i*-th sensor before it is exposed to sample *j*, V_i in the global methods is the original sensor curve response on the *i*-th sensor for all samples, whereas in the local method, $\sum_i V_{ij}^{(k)^2}$ calculated on the *i*-th sensor response for sample *j* only. The baseline difference method can compensate for the effect of temperature because this method eliminates additive errors at the baseline and steady-state responses. The logarithm difference method can linearize the connection between odour concentration and output of the sensor. The local normalization limits the output value of each sensor to one sample from 0 to 1 and is effectively used when the main focus is the identification of odour, not its concentration. In global normalization, the value for each sensor that detects all samples is made in the range 0 to 1. While on the global autoscaling method, the mean of the distribution of the values of each sensor for all samples is made to be zero, and the standard deviation is set to be one [12], [22].

B. Principal Component Analysis (PCA)

PCA is a statistical technique that functions to find patterns in data sets by extracting relevant information from a set of data. PCA reduces complexity and shows the hidden, simple structure behind it. Changes in data dimensions are achieved by transforming data into new bases. In the new bases, noise in the data is filtered out, and important information is revealed [25], [26].

The PCA process algorithm in this study was as follows; first, the sensors' output response was arranged in the form of an $N \times M$ matrix. M was the number of sensors used in the experiment, which is six, while N was the amount of data from one sensor for measuring three samples from 15 data collection, hence, the matrix size was 405×6, and described as matrix A in equation (6)

$$\mathbf{A} = \begin{bmatrix} a_1 & b_1 & c_1 & d_1 & e_1 & f_1 \\ a_2 & b_2 & c_2 & d_2 & e_2 & f_2 \\ & & & \cdot & & \\ & & & \cdot & & \\ & & & \cdot & & \\ a_N & b_N & c_N & d_N & e_N & f_N \end{bmatrix} \quad (6)$$

The second step was to calculate the average value of each sensor response's output. The average value is needed to construct the covarian matrix of A which denoted by **covA**.

The diagonal component of the covariance matrix is the variance of each measurement variable, while the off-diagonal component is the covariance of the variables. Diagonal components are related to data characteristics, while off-diagonal components are related to data redundancy [25]. In order to obtain important data characteristics, it was necessary to manipulate the **covA** matrix by calculating the eigenvector and the eigenvalue of the matrix. The next step was to sort the eigenvector based on the highest to the lowest eigenvalue. The eigenvector with the highest eigenvalue was the first principal component (PC1) of the data set [26]. The plots PC1 and PC2 from the five feature extraction methods are depicted in Fig 4 (a)-(e).

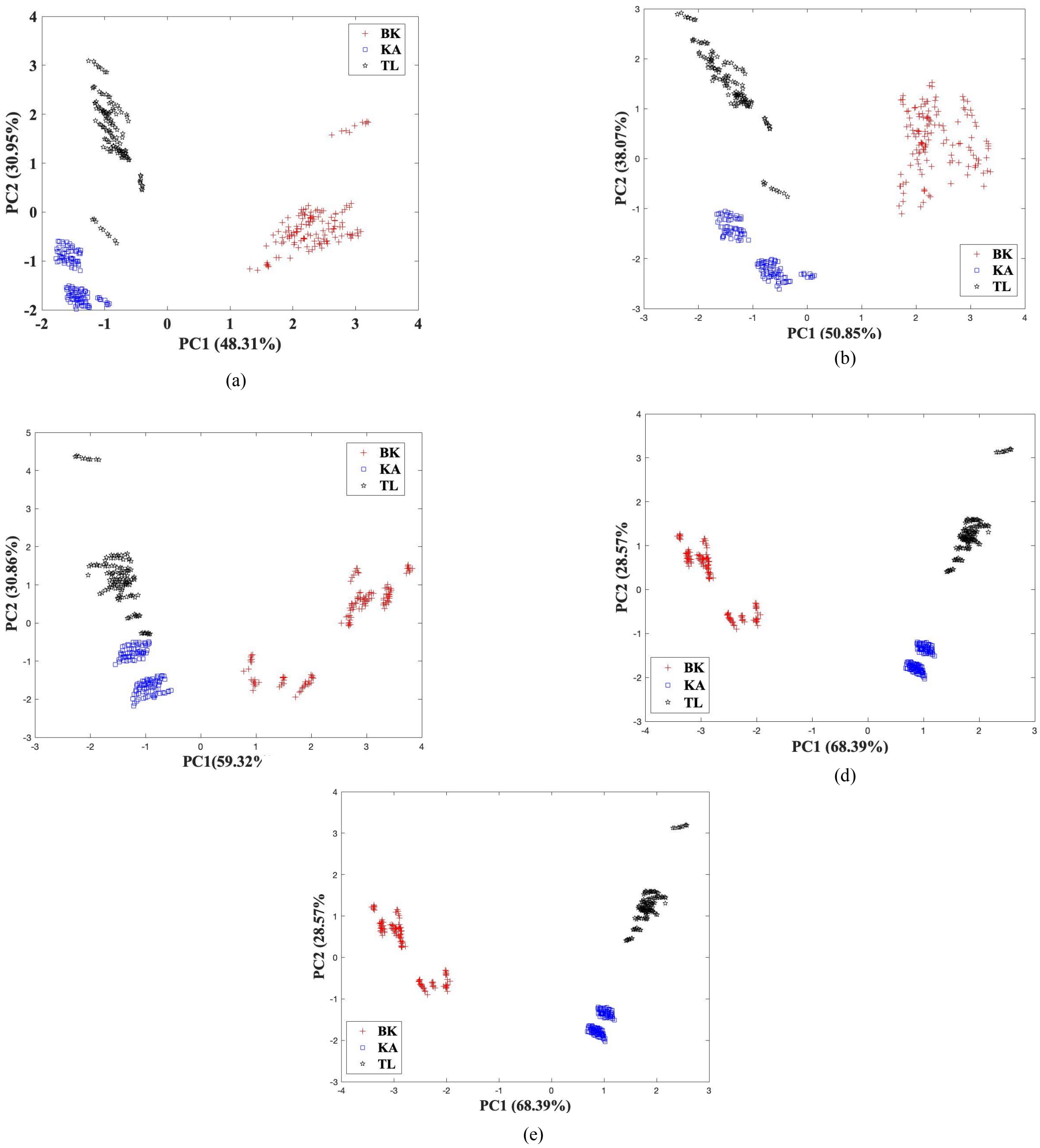

Fig 4. PCA score plots for data samples of *Beras Kencur* (BK), *Kunir Asem* (KA), and *Temu Lawak* (TL) after feature extraction of (a) baseline difference, (b) logarithm difference, (c) local normalization, (d) global normalization, and (e) global autoscaling

Fig 4 shows that clear discrimination was reached for global methods. TABLE II lists the sum of first and second principal components of five different feature extraction methods. From TABLE II, we can see that both global normalization and autoscaling had the highest total sum of PC1 and PC2 that reached 96.96%, followed by local normalization (90.18%), logarithm and baseline difference (88.92 and 79.26%, respectively). To strengthen the result, the feature extracted signal response was also fed into a Backpropagation Neural Network.

TABLE II. COMPARISON OF TOTAL SUM OF 1ST AND 2ND PC FROM FEATURE EXTRACTION METHODS

Feature Extraction Methods	***Total sum of 1st and 2nd PC***
Baseline difference	79.26%
Logarithm difference	88.92%
Local normalization	90.18%
Global normalization	96.96%
Global autoscaling	96.96%

C. Backpropagation Neural Network

The artificial neural network (ANN) is an information processing system that works by imitating the workings of neural networks in the human brain and uses mathematical equations to simulate the learning process and memory. The ANN consists of processing elements in the form of interconnected nodes and works synergistically to solve certain problems. In general, ANNs are modelled with input, hidden layer(s), and output layer. Each node in a layer is related to vertices in another layer by means of a link with a certain weight. These weights reflect the information to solve a problem used by the network. While each neuron is a processing unit that contains an additional and an activation function. Backpropagation is one of the learning algorithms in ANN with trained learning methods. In this algorithm, the training data generates learning rules, and this is used to adjust the weight so that the output is closer to the target [27].

The architecture of the BPNN used in this research is depicted in Fig 5. It consisted of an input layer with six neurons (six sensors), two hidden layers with 25 neurons in each layer, and an output layer with three neurons representing three types of herbal drink. A network training function, Levenberg-Marquardt optimization, was used. The activation function in the first hidden layer was logsig while the second hidden layer and the output layer used the purelin function. From 15 sampling times for each sample, the data used for training was picked from the first and second of data retrieval, and the rest were used for testing. The classification result for BPNN can be seen in TABLE III.

In the BPNN system for the input of sensor response features extracted using the global autoscaling method, almost all of the test data could be recognized; only one data point is misidentified, so the accuracy rate reached 97.44%. Meanwhile, the BPNN network for global normalization, local normalization, logarithm and baseline difference methods has an accuracy rate of 94.87%, 92.31%, 89.74%, and 82.05% respectively. These results are consistent with PCA discrimination, where the highest PC is for the global methods. However, in BPNN, the accuracy of global autoscaling is higher than global normalization. This means that the most suitable feature recognition method is global autoscaling. The method aims to ensure that the sensor magnitude is comparable to the pattern-recognition process.

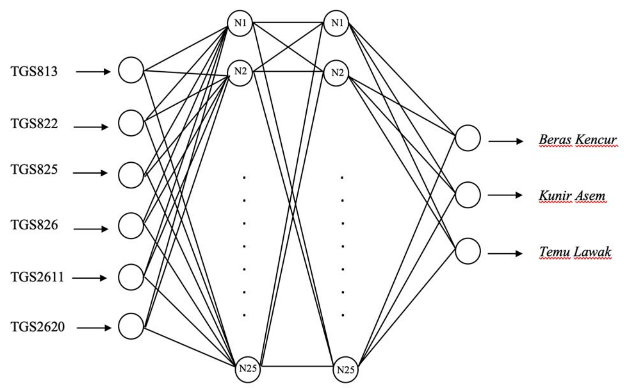

Fig 5. Network architecture of the Backpropagation algorithm

TABLE III. THE ACCURACY OF BPNN OUTPUT WITH FIVE DIFFERENT FEATURE EXTRACTION METHODS AS INPUT

Feature Extraction Methods	***Accuracy***
Baseline difference	82.05%
Logarithm difference	89.74%
Local normalization	92.31%
Global normalization	94.87%
Global autoscaling	97.44%

IV. CONCLUSION

The optimization of the feature extraction method to improve e-nose performance has been investigated. Of the five feature extraction methods, the PCA results show that global autoscaling and normalization provide the best discrimination. This is reinforced by the BPNN analysis, where global autoscaling provides the highest classification results up to 97.44%, and global normalization in the second position with an accuracy rate of 94.87%. This proves that the selection of the feature extraction method affects the e-nose performance results.

ACKNOWLEDGMENT

This work is supported by the Indonesia Endowment Fund for Education (LPDP).

References

[1] G. A. Burlingame, R. L. Doty, and A. M. Dietrich, "Humans as Sensors to Evaluate Drinking Water Taste and Odor: A Review," *J. Am. Water Works Assoc.*, vol. 109, no. 11, pp. 13–24, 2017, doi: 10.5942/jawwa.2017.109.0118.

[2] M. G. Corradini, "Shelf Life of Food Products: From Open Labeling to Real-Time Measurements," *Annu. Rev. Food Sci. Technol.*, vol. 9, no. March, pp. 251–269, 2018, doi: 10.1146/annurev-food-030117-012433.

[3] H. Smyth and D. Cozzolino, "Instrumental methods (Spectroscopy, Electronic Nose, and Tongue) as tools to predict taste and aroma in beverages: Advantages and limitations," *Chem. Rev.*, vol. 113, no. 3, pp. 1429–1440, 2013, doi: 10.1021/cr300076c.

[4] A. Loutfi, S. Coradeschi, G. K. Mani, P. Shankar, and J. B. B. Rayappan, "Electronic noses for food quality: A review," *J. Food Eng.*, vol. 144, pp. 103–111, 2015, doi: 10.1016/j.jfoodeng.2014.07.019.

[5] J. C. Rodriguez Gamboa, E. S. Albarracin E, A. J. da Silva, L. L. de Andrade Lima, and T. A. Tiago, "Wine quality rapid detection using a compact electronic nose system: Application focused on spoilage thresholds by acetic acid," *Lwt*, vol. 108, no. March, pp. 377–384, 2019, doi: 10.1016/j.lwt.2019.03.074.

[6] B. Tudu, B. Kow, N. Bhattacharyya, and R. Bandyopadhyay, "Normalization techniques for gas sensor array as applied to classification for black tea," *Int. J. Smart Sens. Intell. Syst.*, vol. 2, no. 1, pp. 176–189, 2009, doi: 10.21307/ijssis-2017-344.

[7] S. N. Hidayat, A. Rusman, T. Julian, K. Triyana, A. C. A. Veloso, and A. M. Peres, "Electronic nose coupled with linear and nonlinear supervised learning methods for rapid discriminating quality grades of superior java cocoa beans," *Int. J. Intell. Eng. Syst.*, vol. 12, no. 6, pp. 167–176, 2019, doi: 10.22266/ijies2019.1231.16.

[8] S. Labreche, S. Bazzo, S. Cade, and E. Chanie, "Shelf life determination by electronic nose: Application to milk," *Sensors Actuators, B Chem.*, vol. 106, no. 1 SPEC. ISS., pp. 199–206, 2005, doi: 10.1016/j.snb.2004.06.027.

[9] S. Güney and A. Atasoy, "An electronic nose system for assessing horse mackerel freshness," *INISTA 2012 - Int. Symp. Innov. Intell. Syst. Appl.*, pp. 0–4, 2012, doi: 10.1109/INISTA.2012.6246940.

[10] A. Sanaeifar, S. S. Mohtasebi, M. Ghasemi-Varnamkhasti, and M. Siadat, "Application of an electronic nose system coupled with artificial neural network for classification of banana samples during shelf-life process," *Proc. - 2014 Int. Conf. Control. Decis. Inf. Technol. CoDIT 2014*, pp. 753–757, 2014, doi: 10.1109/CoDIT.2014.6996991.

[11] J. Lozano, J. P. Santos, and M. C. Horrillo, *Wine Applications With Electronic Noses*. Elsevier Inc., 2016.

[12] J. Yan *et al.*, "Electronic nose feature extraction methods: A review," *Sensors (Switzerland)*, vol. 15, no. 11, pp. 27804–27831, 2015, doi: 10.3390/s151127804.

[13] S. N. Hidayat and K. Triyana, "Optimized back-propagation combined with radial basic neural network for improving performance of the electronic nose: Case study on the fermentation process of tempeh," *AIP Conf. Proc.*, vol. 1755, 2016, doi: 10.1063/1.4958466.

[14] D. K. Agustika and K. Triyana, "Application of Principal Component Analysis and Discrete Wavelet Transform in Electronic Nose for Herbal Drinks Classification," pp. 6–11.

[15] D. Karakaya, O. Ulucan, and M. Turkan, "Electronic Nose and Its Applications: A Survey," *Int. J. Autom. Comput.*, vol. 17, no. 2, pp. 179–209, 2020, doi: 10.1007/s11633-019-1212-9.

[16] Figaro Engineering Inc., "Technical Information for TGS813." 1999.

[17] Figaro Engineering Inc, "TGS 822 - for the detection of Solvent Vapors.," *Prod. Inf.*, pp. 4–5, 2015.

[18] Figaro Engineering Inc, "TGS 825 - Special Sensor for Hydrogen Gas," *Sensors (Peterborough, NH)*. p. 2, 2004.

[19] Figaro Engineering Inc, "TGS 826 - Ammonia Sensor - MOX sensor," *Prod. Inf.*, 2014.

[20] Figaro USA Inc., "PRODUCT INFORMATION TGS 2611 - for the detection of Methane," *Power*. .

[21] Fígaro USA INC, "TGS 2620 for the detection of Solvent Vapors.," *Prod. Inf.*, 2014.

[22] P. T. C., S. S. S., N. H.T., and G. J.W., *Handbook of Machine Olfaction*. WILEY-VCH, 2003.

[23] J. Fu, G. Li, Y. Qin, and W. J. Freeman, "A pattern recognition method for electronic noses based on an olfactory neural network," *Sensors Actuators, B Chem.*, vol. 125, no. 2, pp. 489–497, 2007, doi: 10.1016/j.snb.2007.02.058.

[24] A. Hierlemann and R. Gutierrez-Osuna, "Higher-order chemical sensing," *Chem. Rev.*, vol. 108, no. 2, pp. 563–613, 2008, doi: 10.1021/cr068116m.

[25] J. Shlens, "A Tutorial on Principal Component Analysis," *ArXiv*, pp. 1–13, 2014, doi: 10.1.1.115.3503.

[26] L. I. Smith, "A tutorial on Principal Components Analysis," *IFAC Proc. Vol.*, vol. 37, no. 1, pp. 511–516, 2002, doi: 10.1016/s1474-6670(17)38783-9.

[27] M. Puig-Arnavat and J. C. Bruno, "Artificial Neural Networks for Thermochemical Conversion of Biomass," *Recent Adv. Thermochem. Convers. Biomass*, pp. 133–156, 2015, doi: 10.1016/B978-0-444-63289-0.00005-3.