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# Detection of decomposition in mahi-mahi, croaker, red snapper, and weakfish using an electronic-nose sensor and chemometric modeling

**Sanjeewa R. Karunathilaka**[1] | **Zachary Ellsworth**[1] | **Betsy Jean Yakes**[2]

[1] Joint Institute for Food Safety and Applied Nutrition, University of Maryland, College Park, Maryland, USA

[2] Center for Food Safety and Applied Nutrition, U.S. Food and Drug Administration, College Park, Maryland, USA

**Correspondence**
Betsy Jean Yakes, 240-402-2720; U.S. Food and Drug Administration, 5001 Campus Drive, College Park, MD 20740, USA.
Email: Betsy.Yakes@fda.hhs.gov

**Abstract:** This study evaluated an electronic-nose (e-nose) sensor in combination with support vector machine (SVM) modeling for predicting the decomposition state of four types of fish fillets: mahi-mahi, croaker, red snapper, and weakfish. The National Seafood Sensory Expert scored fillets were thawed, 10-g portions were weighed into glass jars which were then sealed, and the jars were held at approximately 30°C to allow volatile components to be trapped and available for analysis. The measurement of the sample vial headspace was performed with an e-nose device consisting of nanocomposite, metal oxide semiconductor (MOS), electrochemical, and photoionization sensors. Classification models were then trained based on the sensory grade of each fillet, and the e-nose companion chemometric software identified that eight MOS were the most informative for determining a sensory pass from sensory fail sample. For SVM, the cross-validation (CV) correct classification rates for mahi-mahi, croaker, red snapper, and weakfish were 100%, 100%, 97%, and 97%, respectively. When the SVM prediction performances of the eight MOS were evaluated using a calibration-independent test set of samples, correct classification rates of 93–100% were observed. Based on these results, the e-nose measurements coupled with SVM models were found to be potentially promising for predicting the spoilage of these four fish species.

**Practical Application:** This report describes the application of an electronic-nose sensor as a potential rapid and low-cost screening method for fish spoilage. It could provide regulators and stakeholders with a practical tool to rapidly and accurately assess fish decomposition.

KEYWORDS
electronic-nose, seafood, decomposition, screening

## 1 | INTRODUCTION

Fish are one of the most widely consumed and internationally traded foods in the world today (Tveteras et al., 2019) and are a significant part of our diet as a rich source of premium protein, unsaturated fatty acids, vitamins, and minerals (Wu et al., 2019). The U.S. Food and Drug Administration (FDA) has the primary federal responsibility of seafood safety in the United States (U.S. FDA, 2020), which includes oversight of more than 90% of seafood (by volume) that is imported. Fish is a highly perishable food commodity (Adedeji et al., 2012; Vajdi et al., 2019) with decomposition caused by bacterial decay, enzymatic degradation, and lipid oxidation (Hammond et al., 2002).

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Hence, development of techniques for evaluating freshness attributes of fish is essential (Wu et al., 2019).

For evaluation of seafood freshness, there have been several techniques and methods developed with organoleptic sensory evaluation, the gold-standard for regulation of fish freshness (Cheng et al., 2013; Codex Alimentarius Commission, 1999; Wu et al., 2019). Sensory analysis is fast, simple, and accurate; however, this method requires extensive training to avoid potential subjectivity in analysis (Du et al., 2001; Self et al., 2019). With regard to analytical methods to determine fish spoilage, various volatile compound extraction methods (e.g., solid phase microextraction) combined with chromatographic separation and detection (e.g., GC and HPLC with MS) have yielded accurate results, but these procedures can be laborious, use solvents, require highly skilled operators, and are mostly limited to analytical laboratories (Altieri et al., 2016; Bai et al., 2019; Lee et al., 2018; Lv et al., 2018; Wu et al., 2019). Therefore, there is a need to develop new technologies that can allow for the rapid, simple classification of seafood quality and freshness.

The composition and concentrations of volatiles produced by decomposition due to microbial growth and oxidation of the fish are indicative of the stage of spoilage. One method to detect these volatile compounds is electronic-nose (e-nose) sensor technology. An e-nose instrument commonly consists of an array of sensors that responds to a complex volatile profile with each sensor having a specific affinity toward a chemical (Lee et al., 2018) or, in many cases, individual sensors having overlapping sensitivity for a common class of volatile compounds which then results in a characteristic signature/pattern for each sample (Amari et al., 2006; Di Natale et al., 2001). These sensors have a rapid response to reacting compounds and can be reusable after a short recovery period. Due to these attributes, this technology has been investigated for freshness and authenticity assessment in a wide range of food products such as fruits, vegetables, olive oil, and seafood (Adak & Yumusak, 2016; Buratti et al., 2018; Grassi et al., 2019; Kodogiannis, 2017; Li et al., 2016; Shao et al., 2018; Zhiyi et al., 2017; Zhou et al., 2017). A number of chemometric models have been developed for fish spoilage classification including those of Alaskan pink salmon (Chantarachoti et al., 2006), sardines (Amari et al., 2006), tilapia (Shi et al., 2018), cod (Di Natale et al., 2001), and croaker (Zheng et al., 2016; Zhiyi et al., 2017). The pattern recognition techniques for prediction in these studies included the nonlinear methods of artificial neural network (ANN), support vector machine (SVM), k-nearest neighbor (KNN) (Hasan et al., 2012), and probabilistic neural networks (PNN) (Cheng et al., 2015), as well as the linear method of partial least squares discriminant analysis (PLS-DA) (Grassi et al., 2019).

Despite these successes, e-nose technology has yet to be fully vetted and deployed for seafood decomposition analysis. This is in part due to e-nose technology not allowing compound identification and having a higher detection limit compared to chromatographic methods combined with mass spectrometric detection (Kodogiannis, 2017). Further, e-nose measurement reliability depends on several key factors such as efficient sampling, appropriate selection of sensing elements, optimal data acquisition, proper pre-processing, and suitable pattern recognition modeling (Vajdi et al., 2019). In regard to this, this study seeks to train the classification models based on sensory evaluations performed by U.S. FDA National Seafood Sensory Experts (NSSEs). This allows the chemometric method to generate results which are directly comparable to sensory analysis thus, potentially serving as a more fitting and accurate companion tool. Also, use of appropriate statistical methods to identify informative sensors that are important for a better discrimination of samples is vital prior to the development of classification models. In this case, the e-nose companion chemometric software has a built-in function to identify the informative sensors for this purpose allowing for robust identification of appropriate sensors.

In this study, we evaluated an e-nose sensor, MSEM 160, which is designed for sampling and detection of odors, volatile organic carbons (VOC), and other airborne chemicals. This instrument has a small footprint that could allow the device to be easily portable and deployable for seafood decomposition analysis. This instrument is composed of specific gas sensors for hydrogen sulfide, ammonia, and hydrocarbons, as well as an array of sensors for VOC and other odor causing compounds. This system was evaluated for the classification of fish spoilage in less time and at reduced costs relative to classical analytical techniques. The possibility of classifying fish spoilage using this instrument was evaluated by collecting fish sample data from four different fish types and then performing SVM modeling. The chemometric method was trained using the sensory evaluation scores from NSSEs for fish samples collected from multiple areas of the world and fishing locations. Based on the results, the e-nose-based method was found to be a promising tool in predicting the spoilage of these four fish species.

## 2 | MATERIALS AND METHODS

### 2.1 | Fish samples and sensory analysis

Mahi-mahi (*Coryphaena hippurus*), croaker (*Micropogonias furnieri*), red snapper (*Lutjanus* species), and weakfish (*Macrodon ancylodon*) were evaluated from two

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countries during August and September of 2018 by U.S. FDA NSSEs. Croaker, red snapper, and weakfish were collected from Guyana, and mahi-mahi was collected from Ecuador. Harvest was performed by various vessels in these regions and then the fish were brought to central processing facilities/warehouses in the individual countries where the fish were gutted by hand. On-site NSSEs then performed initial evaluation and controlled decomposition. Natural diversity due to being wild-caught samples led to variability in the age, weight, and length of the samples.

NSSEs are highly trained seafood sensory analysts that undergo the FDA training regime including sensory course participation, training sample set evaluation, and testing. Candidates then serve alongside NSSE experts, preparing training sample sets, providing leadership for the program, training lab analysts, participating in inspections, and other activities relevant to their work, until full qualification is reached. To achieve qualification and NSSE status after their years of rigorous training, candidates must submit a package that is reviewed by current NSSEs and the associated FDA Offices/Centers. Only upon all reviewers agreeing that the candidate is ready and qualified to be an NSSE is the candidate promoted.

In this study, these expert NSSEs identified the fish and performed sensory evaluation and controlled seafood decomposition on-site to create increment-based, scored seafood samples for analytical analysis. Based on sensory assessments by a single NSSE per increment in a set and using established protocols, a sensory score was given to each sample that was related to the intensity and type of the odor. Sensory scores are on a standard 100-point scale where 0 represents the highest possible quality and 100 represents the greatest degree of decomposition. In this scale, seafood is given either a sensory pass or a sensory fail (i.e., 0–49 scores pass while 51–100 scores fail; (Self et al., 2019)). In this manner, depending on a number range on the 100-point scale, samples were assigned to seven different sensory increments (SIs) from 1 to 7. SI values of 1–4 consisted of samples that passed the sensory test with increment 4 being the borderline pass, and SI values of 5–7 consisted of those that failed the test with increment 7 having the most highly decomposed samples. For preparing these increments, freshly caught and gutted fish were first evaluated and given a sensory score based on what was determined for the "freshest" product. These samples then were given the SI 1 designation with additional SI values possible due to natural decomposition from transport and preparation. The remaining fish were then separated into different totes containing ice, representing future SI values, in order to have controlled decomposition. The NSSEs checked the totes every few hours to monitor the decomposition progress. If needed, additional ice was added or ice was removed to control the decomposition process. This process was continued until there were seven increments of decomposition, with fish samples removed at each increment level along the way. Table 1 shows the SI value and associated sensory scores on the 100-point scale along with sensory descriptions for the samples evaluated in this study.

After grading and achieving the desired SI increment, all the samples in the fillet form were immediately individually packaged in sterile vacuum packs, labeled with the corresponding SI number, and frozen. Fish skin was left on the samples for croaker, red snapper, and weakfish, while the skin had been previously removed from the mahi-mahi samples. Frozen samples were received at our lab in the sterile vacuum packs that had been shipped on ice. Samples were immediately stored at −20 °C until prepared for analysis.

## 2.2 | Sample preparation and e-nose measurement

The MSEM 160 (Sensigent LLC, Baldwin Park, CA, USA) portable multi-sensor environmental monitor was used to analyze the volatile compounds from the four fish species. The MSEM 160 sensor is equipped with an array of 32 gas sensors including temperature (sensor 1), humidity (sensor 2), metal oxide semiconductor sensors (MOS: sensors 5–12), electrochemical (EC: sensor 13 ($H_2S$), sensor 14 ($NH_3$), sensor 15 (hydrocarbon)), photoionization (PI: sensor 16 (total volatile organic carbon (TVOC))), and polymer composite (PCS: sensors 17–32) sensors. Sensors 3 (additional temperature) and 4 (additional humidity) were inactive for this study which left 30 sensors for data collection. In its fully configured format, the device is 12 cm high × 18 cm wide × 20 cm deep and contains wireless communications which could allow for portable measurements. While the instrument contains a small on-board screen and internal computer for full portability, an externally connected monitor and keyboard/mouse were used during this method development research.

At the beginning of each day of data collection, the instrument was turned on for an hour to stabilize the sensor responses. Prior to the data collection, a sample (randomized with respect to increment number) was taken out of the freezer, the fillet immediately crushed into pieces (with the skin if containing), the flesh weighed into two 10 g portions, and each portion placed in a separate 250-mL wide-mouth septa jar that was sealed with a PTFE/silicone septum-containing screw cap (Fisher Scientific, Waltham, MA, USA). The jars were used as-is from the manufacturer and were not reused during these exploratory studies in order to eliminate potential variability from cleaning. The jars were placed in an approximately 30 °C oven

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**TABLE 1** NSSE sensory information for the seafood samples evaluated in this study

| Sensory increment | Sensory scores and NSSE comments (when available) | | | |
|---|---|---|---|---|
| | Mahi-Mahi | Croaker | Red snapper | Weakfish |
| 1 – Pass, most fresh | 15–20 | 20+, Pondy | 20–25, Citrus | 20+, Briny |
| 2 – Pass | 25–30 | 24–25, Neutral | 25–30, Neutral | 25–30, Neutral |
| 3 – Pass | 30–40 | 30–35, Stale | 30–35, Stale | 30–35, Stale |
| 4 – Borderline pass | 45+ | 40–45, Oxidized/fishy | 45+, Strong stale | 40–45, Oxidized |
| 5 – Borderline fail | 55–60 | 55–65, Sour | 55-60, Sour | 55–60, Slight sour |
| 6 – Fail | 65–70 | 65–70, Strong sour | 60-70, Strong sour | 65–70, Sour |
| 7 – Fail, most decomposed | 75+ | 70+, Garbage | 70+, Yeasty | 68–75, Strong sour/fermented |

for 40 min to allow for headspace equilibration. A 3 ¼ inch needle (gauge size 14) was coupled to the MSEM sampling and exhaust ports via 1/8 inch ID Tygon tubing and Luer lock connections in order to draw-in/exhaust the headspace gas to/from septa jars. The instrument flow rate was 450 mL/min, and the data acquisition rate was 1 s. The instrument was operated in Triggered Mode for acquisition which consists of three stages: pre-sample purge, sample, and post-sample purge. For the seafood sample analysis these were set to: (1) 90 s pre-sample baseline purge during which carbon-filtered ambient air was passed through the sensors; (2) 90 s sample draw during which the headspace of the sample was drawn through the sample port, and the exhaust from the MSEM was connected back into the container jar to form a closed-loop system; and (3) 90 s post-sample purge during which carbon-filtered ambient air was passed through the sensors. Additionally, a clean air cycle (180 s) to purge the system was performed before each sample measurement. This equates to a total of approximately 7.5 min per sample measurement cycle.

The raw sensor readings for each sample were saved in .CSV file format. The raw sensor data files were then pre-processed using the CDAnalysis software (Version 11.2, Sensigent LLC) prior to the application of a pattern recognition algorithm. For each sample measurement, the $\Delta R/R$ value was computed, as the change in resistance from a baseline value prior to the start of the sample exposure ($\Delta R$) which was then divided by the baseline value (R). Thirty-two (4 fillets for each SI 1–7 plus 3 more fillets, respectively, from SI 3 and 5) mahi-mahi, 35 (5 fillets for each SI 1–7) croaker and red snapper, and 34 weakfish (5 fillets for each SI 1 and 3–7, 4 fillets for SI 2) samples were used for the e-nose data collections. Duplicate measurements were collected from two separate portions of a fillet. Due to data collection issues, data files for 3 red snapper, and one croaker and one weakfish were not available, thus leaving 64, 69, 67, 67, total measurements for mahi-mahi, croaker, red snapper, and weakfish, respectively, for model development.

## 2.3 | Multivariate data analysis

The e-nose data were analyzed by two different chemometric tools for data exploration and/or classification. Principal component analysis (PCA) and SVM were performed using PLS_Toolbox chemometric software (version 8.6.1, Eigenvector Research Inc., Wenatchee, WA, USA) and Sensigent's Chemometric Data Analysis (CDAnalysis) software. Different pre-processing methods such as Savitsky–Golay (Sav–Gol) using a first-order polynomial fit, baseline correction, and area normalization, alone or in combination, were applied to the raw sensor data to remove artifacts such as high and low frequency noise, to improve the signal-to-noise (S/N) ratio, and to correct for the effect of changing sensor response baselines during measurement. The optimum pre-processing method/combination was selected based on the highest correct classification rates provided by the pattern recognition algorithm.

PCA was implemented as a data exploration and visualization tool. PCA reduces the dimensionality from many sensor responses (here 30 sensors), to a much smaller set of principal components (PCs). The first principal component (PC1) captures the largest possible variance in the data, while each succeeding component (PC2, PC3, etc.) captures the next largest variances. Often two or three principal components provide an adequate representation of the data which is most commonly presented on a PCA scores plot (Karunathilaka et al., 2016). In this study, PCA was used to explore the possibility of differentiating the samples that failed the sensory evaluation (SIs 5–7) from those that passed (SIs 1–4) and to identify the most informative sensors that best discriminated between these two sample groups.

SVM is a well-known supervised classification approach that is particularly useful for overlapping or poorly resolved complex data sets with inherent nonlinearity. In SVM, the input data are first mapped into a high dimensional space using a kernel function, and then samples are separated into different classes using a hyperplane

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**TABLE 2** Support vector machine (SVM) classification results for the models developed for the e-nose sensor data obtained for four species of fish. Results are shown for the prediction of a calibration-independent set of test samples

| Fish type | Test set | # of class samples | Test set (predicted) | |
|---|---|---|---|---|
| | | | SI 1–4 | SI 5–7 |
| Mahi-mahi | **SI 1—4** | 16 | 16 | 0 |
| | **SI 5—7** | 12 | 0 | 12 |
| Croaker | **SI 1—4** | 16 | 16 | 0 |
| | **SI 5—7** | 12 | 0 | 12 |
| Red snapper | **SI 1—4** | 16 | 16 | 0 |
| | **SI 5—7** | 12 | 1 | 11 |
| Weakfish | **SI 1—4** | 16 | 16 | 0 |
| | **SI 5—7** | 12 | 2 | 10 |

decision surface (Karunathilaka et al., 2020). Using a leave-one-out cross-validation (LOO-CV) algorithm, CDAnalysis finds the optimum kernel width in classification model development. The performance of SVM models were evaluated both based on a LOO-CV and by using a calibration-independent test set of samples. For test set prediction, the total data set of a fish species was randomly partitioned into a training set and a test set. Training models were developed using 36 (SIs 1–4 = 18 and 5–7 = 18) samples for mahi-mahi, 41 (SIs 1–4 = 23 and 5–7 = 18) for croaker, 39 (SIs 1–4 = 24 and 5–7 = 15) for red snapper, and 39 (SIs 1–4 = 21 and 5–7 = 18) for weakfish. The remaining samples of each fish type were used for prediction (Table 2).

## 3 | RESULTS AND DISCUSSION

### 3.1 | Principal component analysis

PCA was performed as a way to visually evaluate the possibility of differentiating fish samples that failed the sensory evaluation from those that passed. In many e-nose applications, not all the sensors are important for discrimination due to the specific volatiles evaluated and their interactions with the various sensors. Including non-informative sensors could contribute noise to the supervised classification methods thus increasing the classification error and lowering the predictive capability. The sensors that are most effective for discriminating the two types of samples were identified using the instrument-dedicated CDAnalysis software. CDAnalysis uses "Importance Index (II)" (also called discrimination power (Robotti & Marengo, 2016)) to determine sensor contribution. The sensors with higher II values are effective for discriminating the analytes in the training set. Initial PC analysis using all 30 active sensors was performed and based on a default threshold value of 1.5 for II, MO sensors 5–12 were found to be the most effective for discriminating between sensory passed versus failed samples. These eight sensors had II values higher than that of the default threshold value whereas the other sensors had comparatively lower values (less than 1).

The selection of MOS as the informative sensor from this study was consistent with the literature reports that indicated that the MOS were the most widely used EN technique for fish freshness assessment (Wu et al., 2019). In e-nose, each sensor has a unique sensitivity and selectivity profile. As a group, their responses give a unique pattern for the volatile organic headspace compounds of the test sample (Di Natale et al., 2001; Green et al., 2011). The sensor responses, normalized to the highest response, collected during the sample purge cycle for these eight informative MO sensors are shown in Figure 1a–d and supplemental Figure 1a–d for representative measurements collected from croaker fillets (one sample each from SIs 1–7). For the MOS sensors, upon "smelling" each sample, the e-nose response decreased over time as the volatiles produced by the sample were analyzed. The more decomposed samples (black, red, and purple lines) showed a greater decrease from the initial baseline prior to reaching steady state than the sensory pass samples (green, blue, yellow, and pink lines). E-nose responses, however, were not completely linear with the corresponding sensory increment number, especially for SIs 1–4.

PCA was then performed using only the informative sensors (MO sensors 5–12) to explore the possibility of better differentiating between two classes of samples (sensory test passed vs. failed). Figure 2a–d show the PCA scores of the first two components which explained 95.6%, 97.3%, 97.0%, and 93.6% of the cumulative variances of mahi-mahi, croaker, red snapper, and weakfish data, respectively. Discrimination between the two types of sample groups was observed for all four types of fish (Figure 2a–d), as seen in the NSSE passed samples (blue dots) having clustering generally separated from the NSSE failed

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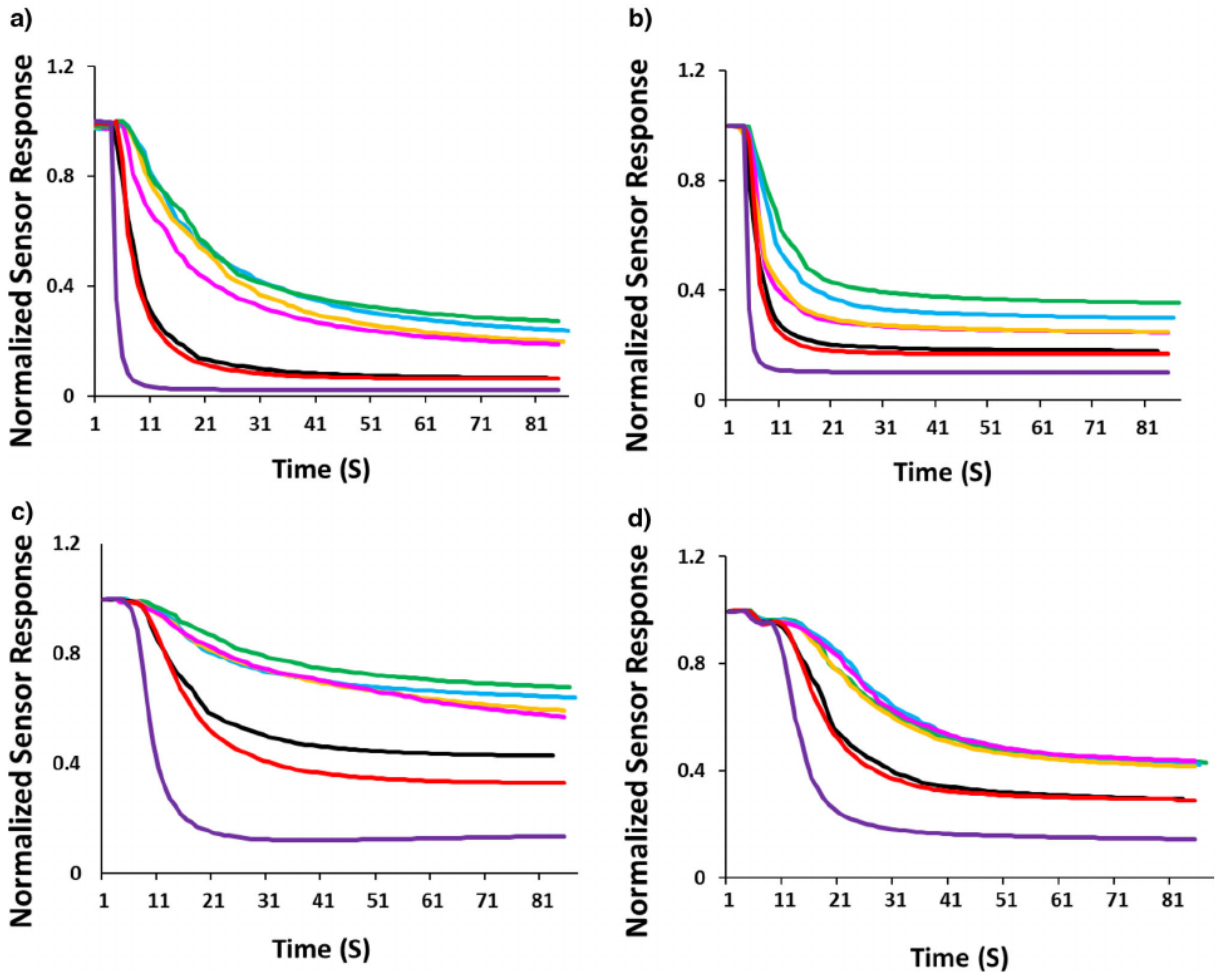


**FIGURE 1** Representative e-nose sensor response for croaker measurements from four sensors: (a) MO sensor 5, (b) MO sensor 6, (c) MO sensor 7, and (d) MO sensor 8. The line colors of green, blue, yellow, pink, black, red, and purple correspond to responses from SIs 1–7, respectively

samples (red squares). SIs 1–4 were clustered together in the positive side of the PC1, while those of 5–7 were clustered together in the negative side. Generally, SI 7 had the most negative PC score values (for clarity, representative labeled in Figure 2a–d), hence, were located furthest away from the cluster for SIs 1–4. This is consistent with the sensor responses observed in Figure 1a–d and supplemental Figure 1a–d where the most decomposed samples (SI 7) had the lowest sensor responses.

From these plots, it appears that the degree of discrimination is dependent upon the fish type. This indicates that a specific classification model for each fish species would be needed for better discrimination between the two types of samples (i.e., a universal model that combines all fish types together would be less sensitive). These finding were consistent with similar studies by Mai et al. (2009) and El Barbri et al. (2008) who have reported that fresh fish clustered on one side of PC1, and, with storage time, the data moved to the other side of the PC. This observed negative correlation of PC scores with SI number is consistent with the observed sensor responses (Figure 1a–d and supplement Figures 1a–d) in which the responses showed greater decrease for the more decomposed samples. Based on these findings, the e-nose appeared to be a promising tool in detecting fish spoilage, and, due to the nonlinearity of the sensor responses, the nonlinear pattern recognition method SVM was applied to further discriminate the samples.

## 3.2 | Support vector machine classification

The FDA classifies seafood samples as decomposed (fail) or non-decomposed (pass) for safety determination. Therefore, the initial target of the e-nose classification

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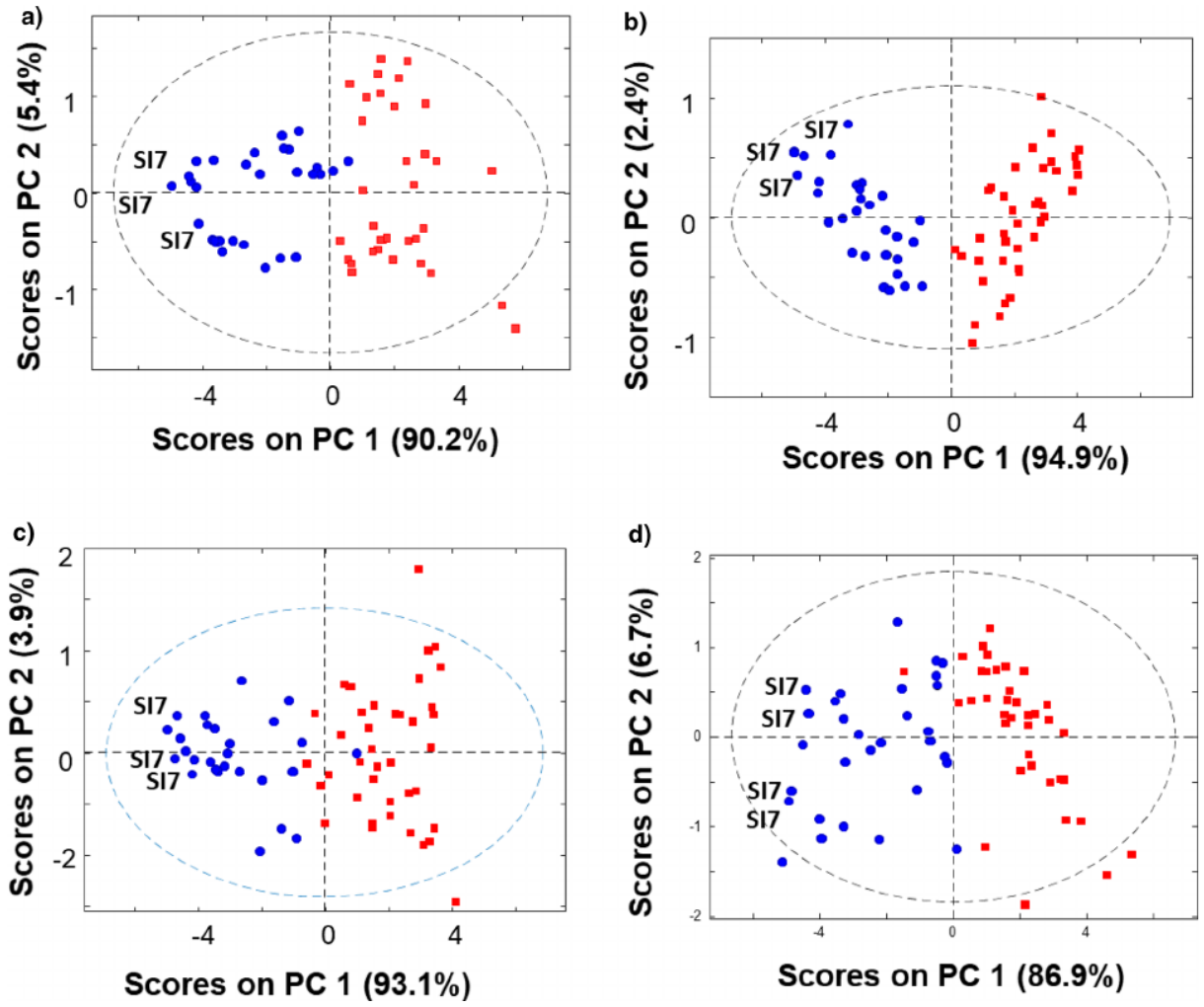


**FIGURE 2** Unsupervised PCA score plots of the e-nose data collected from the 8 informative MO sensors for (a) mahi-mahi, (b) croaker, (c) red snapper, and (d) weakfish. In each plot, the sensory passed samples (SI 1–4) are shown as red squares while the sensory failed samples (SI 5–7) are shown as blue circles. Representative SI 7 points are labeled to show position on the plots. The black dotted circle represents the 95% confidence line for PC scores

methodology using SVM was designed to demonstrate this capability. SVM classification models were developed separately for each fish species using the CDAnalysis software in order to discriminate samples that failed the sensory evaluation (SI 5–7) from those that passed (SI 1–4). SVM models were developed using only the eight informative MOS sensors indicated from the PC analysis. Sav–Gol smoothing filter with or without baseline correction followed by an area normalization was evaluated, and Sav–Gol smoothing filter alone was found to be the optimum data pre-processing method based on the highest correct classification rates for all fish types except for mahi-mahi. Raw data for mahi-mahi were preprocessed using Sav–Gol smoothing followed by a baseline correction and an area normalization. PCA was applied to visualize the SVM cross-validation class boundaries in two dimensions as shown in Figure 3a–d where the yellow circles represent the sensory test passed samples while the green squares represent the sensory test failed samples. Figure 3a,b show a 100% correct classification with all sensory test passed samples on the left side of the separating boundary (blue line) while those that failed the sensory test were on the right side. One misclassified sensory test failed sample (green square among the yellow circles, Figure 3c) and a misclassified sensory test passed samples (yellow circle among the green squares, Figure 3d) were observed. The percentage correct classification rates from cross-validation were then evaluated. For CV, the SVM predicted percentage correct classification percentage rates were 100, 100, 97, and 97 for mahi-mahi, croaker, red snapper, and weakfish data, respectively. High accuracy in predicting the sensory evaluation passed versus failed

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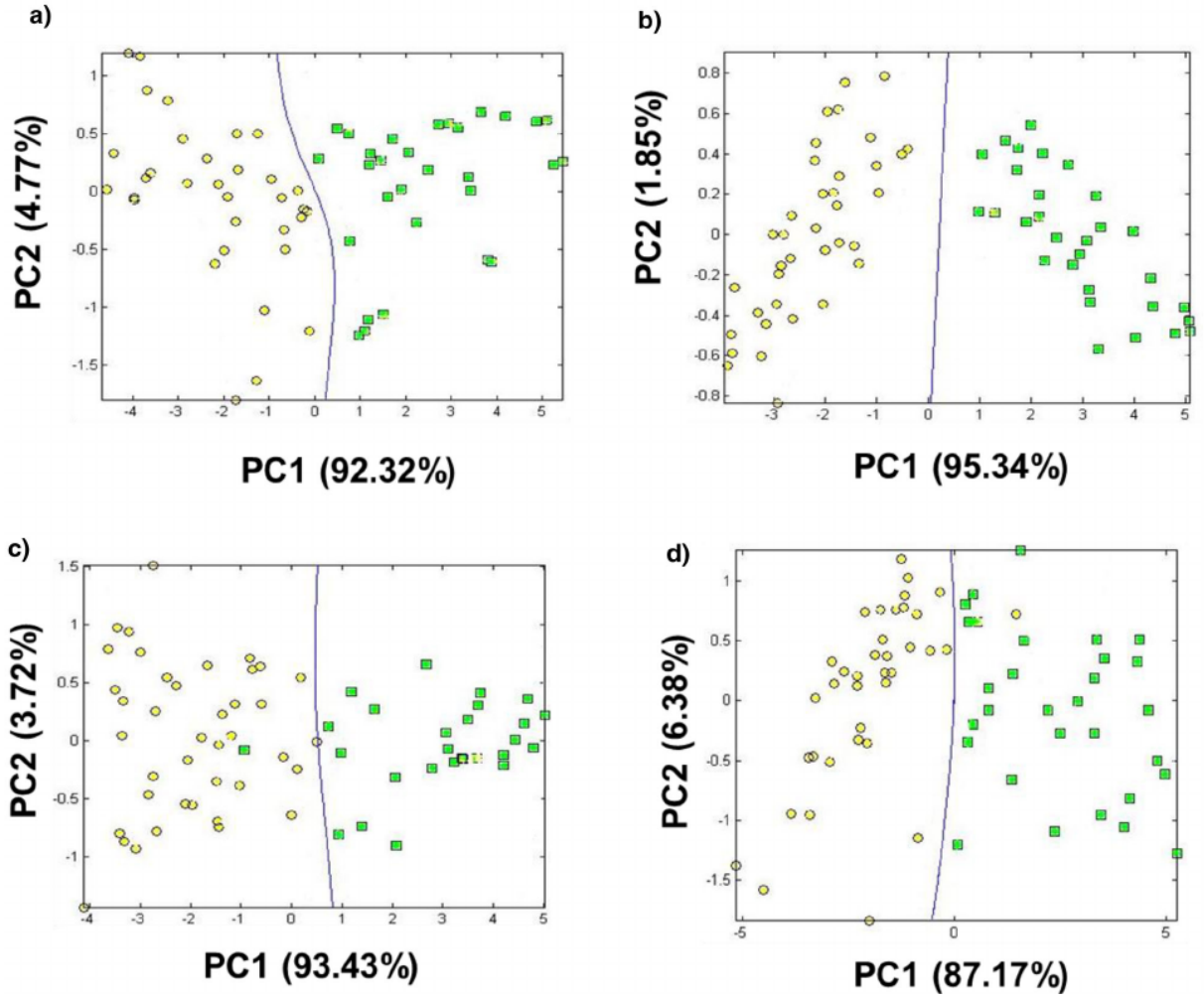


**FIGURE 3** SVM cross-validation results for (a) mahi-mahi, (b) croaker, (c) red snapper, and (d) weakfish. PCA was used to visualize the SVM class boundaries (blue line in just two dimensions). In each plot, the sensory passed samples (SI 1–4) are shown as yellow circles while the sensory failed samples (SI 5–7) are shown as green squares

samples was observed, as the correct classifications were 97% or greater for each fish species.

The prediction performance of sensor-SVM combined method was further evaluated by training an SVM model and testing the prediction performance using a calibration-independent set of samples. The prediction performances of the four SVM models developed for each fish type are shown in Table 2. 100% correct classification rate was observed for both mahi-mahi and croaker data. However, one red snapper and two weakfish sensory evaluation spoiled samples were incorrectly classified as "passing" based on the SVM classification (Table 2) resulting in correct classification rates of 96% for red snapper and 93% for weakfish. These incorrectly classified samples were from SI 5. This increment was samples that were just above the level considered fit for human consumption, and these samples were close to the classification threshold thus making it challenging to have full separation based on the positioning of the separating surface between the data classes. Overall, this combined method was found to be accurate in classifying passed/failed samples with 93–100% correct classification rates for the four species evaluated in this study.

Similar work using e-nose systems, but without controlled lab degradation and NSSE scoring, has shown comparable results to those here-in. El Barbri et al. (2008) used a portable e-nose system with MOS and chemometric modeling to evaluate freshness of Moroccan sardines. In this work, the fish were aged at 4°C, and the accuracy with regard to predication of storage days and associated freshness was 93.75%. Chantarachoti and colleagues also employed a portable e-nose detector to evaluate lab-aged, whole salmon samples, with correct classification rates of 85% and 92% for belly cavity volatiles for samples held

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at 14°C for up to 3 days and slush ice for up to 16 days, respectively (Chantarachoti et al., 2006). Interestingly, the authors note that improvements in the method could be made by using more diverse samples, such as varied harvest times and species, along with studying instrument reproducibility and repeatability, in order to fully employ the device. In this work, by combining both gold-standard NSSE-graded samples along with diversity in species and multiple days of analysis, the use of e-nose technology has been further vetted.

In this work, a classification method to discriminate sensory-analyzed pass samples from failed ones was developed using the data collected from an e-nose sensor. This developed method can be used to classify fish spoilage with the potential for reduced costs, simplicity, and without the use of any chemicals with respect to other analytical methods. However, several steps in the experimental setup need to be further evaluated to improve upon the sample preparation and data acquisition for potential field deployment. In the current settings, samples were kept at an elevated temperature for 40 min in 250 mL jars to equilibrate the headspace. In field applications, however, it would be beneficial to have an efficient sampling protocol with a shorter equilibration time that uses a smaller sized vessel or a sniffer accessory. Additionally, in the current instrumental design, there is no integrated chemometric software in the device for pattern recognition which necessitates data file transfer and off-line data analysis. Further investigations into the need for models for each fish species are being evaluated, as well as evaluation of the natural diversity (e.g., subspecies, geographical region of fishing, fishing season) to understand these effects on the models. Finally, studies to assess the ability to transfer models and instrument-to-instrument variability would be needed for full deployment.

## 4 | CONCLUSION

Here we report the development of a simple and accurate method to detect fish decomposition based on data collected by using an e-nose sensor and the application of a pattern recognition algorithm. A headspace sampling method was developed and employed in a laboratory setting. Sensor array data coupled with PCA could be used to visually distinguish between the NSSE evaluated passed versus failed samples. Eight MOS sensors were found to be the most important for discrimination of decomposition. The prediction performance based on an internal validation based on CV and an external test set prediction indicated that classification models built for the e-nose data can detect fish decomposition with high accuracy. For CV, the SVM correct classification rates were 97–100% for the four species of fish, and 93–100% correct classification rates were observed for the prediction of the test sets of samples with failing samples only at the borderline pass/fail boundary. Future studies will include the development of a more efficient sampling method to determine the capability of the e-nose in predicting fish decomposition during field applications.

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## AUTHOR CONTRIBUTIONS

Sanjeewa Ranasinghe: Conceptualization; Data curation; Investigation; Writing-original draft; Writing-review & editing. Zachary Ellsworth: Data curation; Investigation; Writing-review & editing. Betsy Jean Yakes: Conceptualization; Data curation; Investigation; Project administration; Supervision; Writing-review & editing.

## CONFLICT OF INTEREST

Theauthors declare no conflict of interest.

## ORCID

*Betsy Jean Yakes* https://orcid.org/0000-0003-2457-1855

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## SUPPORTING INFORMATION

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