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Using artificial intelligence to develop a VOC multi-gas sensor system for detecting air quality in shopping centres

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Abstract: With the increasing awareness concerning indoor air quality (IAQ) and energy efficiency, the development of IAQ sensor systems is becoming more relevant, for example to enable demand-controlled ventilation (DCV). Currently, DCV in most indoor environments is based on CO_2 concentration, which is a good indicator for human emissions. For shopping centres (SC), DCV rarely considers volatile organic compound (VOC) emissions from materials, which could significantly affect customer health and consumer experience. VOC multi-gas sensor systems (VOC MGSS) can help to detect and interpret these gases. Due to the high number of sensors and influencing factors such as temperature, relative humidity or type of odour, choosing the best model approach for evaluating IAQ is not trivial. Therefore, we compare linear regression with support vector regression, artificial neural networks and random forest models for the calibration of a VOC-MGSS to predict perceived intensity (PI) for six different SC products. Subjective test data from a trained subject panel and objective test data from the VOC-MGSS are used to train the different model types for the overall dataset and product-specific (PS) datasets.

Keywords: Indoor air quality, total volatile organic compounds, artificial intelligence, E-Nose, linear regression, support vector regression, artificial neural networks, random forest regression

1. Introduction

Several studies show the impact of indoor air quality (IAQ) among others on human health, occupant well-being, comfort and productivity and consequently the need for efficient ventilation strategies [1]. One way of achieving high IAQ with low energy requirements is to use demand-controlled ventilation (DCV). Currently, DCV is mostly based on CO_2 concentration, which is a good indicator of human emissions. However, in SC releasing potentially hazardous VOC from seemingly harmless sources is proven to cause high potential risk to human health, causing sick-building syndrome (SBS) or building-related illnesses [2]. Thus, identification of VOC-inducing products and correlation to subjective evaluation data are essential for a healthy and comfortable environment in SC.

Compared to expensive and complex to use gas chromatography-mass spectrometry, VOC-MGSS are cheap and convenient testing methods to detect VOCs in indoor environments [3, 4]. For such VOC-MGSS, different sensor types can be used. An often-used sensor type is the metal oxide semiconductor (MOx) sensor. Among other benefits being high sensitivity to low gas concentrations, long service life and a low price, MOx sensors are potentially suitable for use in DCV systems. Examples of VOC-MGSS with MOx sensors are available for research use, such as KAMINA from the Karlsruher Institute of Technology (KIT) [5] and for commercial use, such as i-Pen, PEN2, and PEN3 from Airsense Analytics [3] to assess air quality in indoor areas.

Since most of these devices have data from more than one sensor, implementing an artificial intelligence framework can be used to correlate the output of all sensors with target variables, for example to distinguish between different odours or to predict perceived intensities. Earlier research combines artificial intelligence methods and VOC-MGSS technology successfully. Soh et al applied artificial neural networks (ANNs) for herbs recognition [7]. The accuracy of the model reaches 90% in the best case. Wang et al. used a random forest (RF) model for the concentration prediction of binary mixed gases, with the model having an R^2 score of 0.98 [8].

For the assessment of SC air quality, we already developed an VOC-MGSS mainly based on MOx sensors [6]. Different SC product types were tested with the VOC-MGSS and a trained subject panel to evaluate the PI. This testing aimed to find a correlation between objective and subjective data. In this previous work, only one sensor within the VOC-MGSS system was investigated and linear regression analysis was used [6]. For improved analysis, our goal is to investigate different AI frameworks for this application and find the most sufficient model that will enable the VOC-MGSS system to apply all its sensors when calculating the PI.

Table 1. *Sensors and detectable gases within VOC-MGSS system.*

Sensor	Detectable gases
MQ-2	Hydrogen, methane, propane, i-butane, LPG , alcohol, smoke
MQ-3	Alcohol, ethanol, smoke
MQ-7	Carbon monoxide
MQ-9	Carbon monoxide, flammable gasses
MQ-135	Ammonia, nitrogen oxide, alcohol, benzene, smoke, carbon dioxide
HCHO	Benzene, toluene, alcohol, formaldehyde gas, hydrogen
BME680	Industrial sensor for TVOCs

2. Methods

2.1 Objective and Subjective tests

The preceding study was conducted in the Air Quality Laboratory of the EBC. The SC product groups were divided into six categories: books, shoes, clothing, coffee and two perfume variants (100% and 40% diluted). These were filled into so-called emission chambers, shown in **Figure 1**. The chambers are connected to an HVAC system to ensure constant temperature and humidity. Inside each chamber beside the product, the VOC-MGSS was positioned to detect the VOC emissions from the products. A more detailed description can be found in [6].

The essential component within the developed VOC-MGSS system is a MOx sensor array of the MQ sensor series, which can detect a range of VOCs. The MQ sensors were manually pre-calibrated by adjustment of the potentiometer and post-calibrated to temperature and humidity with respect to the log curves available in the datasheets. All applied sensors in this system are outlined in **Table 1**. The VOC-MGSS prototype, including optimized housing, can be seen in **Figure 2**.

Figure 1. Emission chambers in the Air Quality Laboratory at EBC.

Figure 2. VOC-MGSS prototype of EBC, RWTH Aachen University.

For subjective evaluation of the emission intensity from the SC products, a trained panel consisting of 17 participants aided with an acetone test stand was used according to DIN ISO 16000-28. The conducted tests ran with a comparative acetone scale ranging from 0 to 28 PI.

The tests were carried out in respect with variations in temperature (20, 23, 27 °C), relative humidity (30, 50 %) and the air change rate (1, 1.7, 2.05, 3.15, 4.1, 5.1 h^{-1}). In total, 36 evaluations per product and test subject were recorded and stored in a dataset.

2.2 AI Model development procedure

To find a suitable model to predict the perceived intensity depending on the sensor data, different AI models were created and assessed on the MATLAB Regression Learner App. This GUI allows for training, validation, and tuning of models. In our context, sensor signals in **Table 1** are categorized as input data, also called predictors, while the corresponding perceived intensity is the known response. External factors are excluded from predictor selection as an ideal sensor calibration is assumed.

Despite all model types operating differently, the developing approach for each model type is similar, which can be mainly divided into a training and testing process. The model developing procedure for the AI models (AI MDP) is shown in **Figure 3**.

2.2.1 Dataset pre-processing

After a random permutation of the dataset it is separated into training and testing datasets by using 80/20 split [12]. The following step is setting specific model parameters and training of the model with the training dataset. Cross-validation values are calculated to determine the training success[13]. Finally, the trained models are tested to evaluate their performance. To investigate if a product specific (PS) model development leads to improvements in the predictions of the different model types, AI MDP is applied for overall data and each product separately. This leads to six additional product specific models for each model type.

2.2.2 AI model setup

AI models significantly differ in behaviour, algorithmic concept and general bias/variance relevance for different model types in traditional AI problem-solving, machine learning, and deep learning applications [14]. For this, four model types were tested to evaluate their suitability, see **Figure 3**.

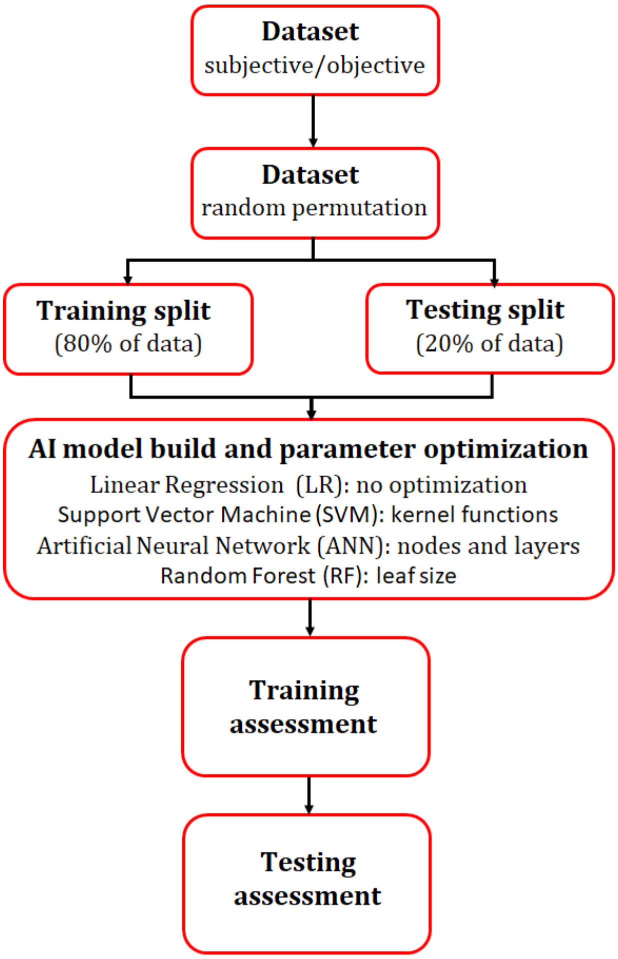

Figure 3. AI model development procedure (AI MDP).

Linear regression finds the best parameter fitting for a regression function with the determination of RMSE. Despite its simplicity, it is subject to underfitting and is affected by outliers [15].

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n \tag{1}$$

Equation (1) shows the applied linear regression function. In this study, y is the predicted perceived intensity, β_n are the fitted coefficients and x_n are the predictors.

Support vector machine (SVM) regression involves the addition of support vectors and kernel functions to estimate a target function within a set constraint (ε) and eliminate outliers (ϑ) from its analysis. The kernel functions can include higher polynomials in finding an optimal hyperplane. In our case, linear and quadratic models are considered. However, the disadvantage is in optimizing the constraint (ε), which can cause a high error tolerance [16]. **Figure 4** visualizes the regression process of a support vector machine with MQ-2 sensor data from this study.

As our system includes multiple MQ sensors more complex models in ANN can run those through numbered sets of layers and nodes[17]. In this study, two network configurations of one layer and 25 nodes and two layers with ten nodes each are used. The main advantage of ANNs is in detecting all possible interaction between predictors. Despite this, ANNs can easily over-fit, and require great computational resources [18, 19]. **Figure 5** visualizes an example of an ANN with sensor signals as inputs, the PI prediction as its output.

Encompassing the same idea with a different execution is random forest (RF) algorithms. Here, the general aim is within constructing a number of decision trees for training [20]. These trees operate with leaves representing data values and applying binary thinking. The leaf size (LS) is related to the number of observations considered in each data split. Thus, RF models with small (4) and large (36) LS were applied in our case. The benefits of RF models are their robustness against outliers. In contrast to this, they are affected by small changes in data [15]. An example of a random forest model is seen in **Figure 6**.

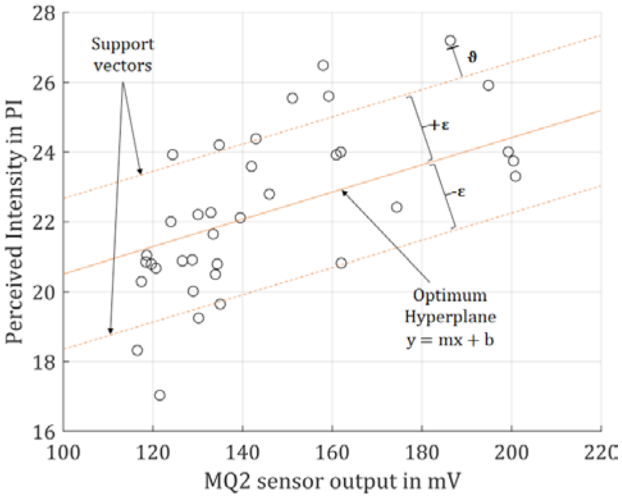

Figure 4. Sample prediction of perceived intensity using support vector regression with MQ-2 sensor output.

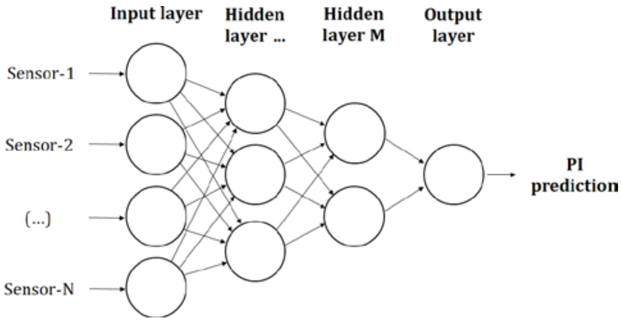

Figure 5. Simplified artificial neural network (ANN) structure in application with VOC-MGSS input & output data.

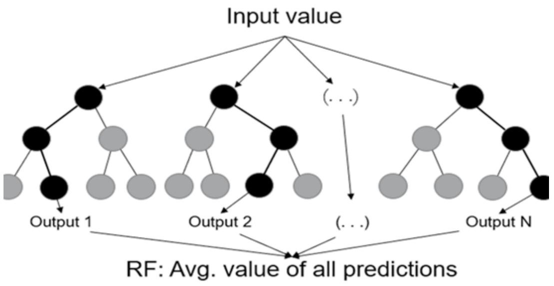

Figure 6. Simplified visualization of random forest algorithms.

2.2.3 Model testing

To build models that accurately predict the PI from objective data, evaluation of the suitability of each model to the dataset is required. RMSE shows how much the model predictions deviate from the subjective test data. [21]. Equation (2) shows the definition for the RMSE. In this study, y_i is PI of the subject test, $m_i\,(AI)$ is the prediction of each model and n represents the number of data values.

$$\text{RMSE (AI)} = \sqrt{\frac{1}{n} \cdot \sum\nolimits_{i=1}^{n} \left(m_i(AI) - y_i \right)^2} \qquad (2)$$

3. Results

3.1 Training and testing of the overall model

Table 2 presents the RMSE for training and testing for the whole dataset. **Figure 7** shows no major differences in the distribution of the data between the subjective test (red boxplot) and LR, ANN, RF and Quadratic SVM models (grey boxplot), only a small difference is observed for Linear SVM. **Table 2** shows the best performance for the RF model with a leaf size of 4 and 36, achieving testing RMSE of 0.07 and 0.75 PI respectively. The ANN models (1x25 and 2x10) also show a good performance, achieving testing RMSE of 0.85 and 0.86 PI.

Table 2. *Resulting training and testing RMSE for the overall models.*

AI model	RMSE in PI Training	RMSE in PI Testing
Linear Regression	2.15	2.12
Linear SVM regression	2.14	2.15
Quadratic SVM regression	1.24	1.84
ANN (2x10)	2.48	0.86
ANN (1x25)	1.01	0.85
RF (leaf size: 4)	0.10	0.07
RF (leaf size: 36)	0.80	0.75

3.2 Testing of the product specific models

Figure 8 shows the RMSE for the overall models (red bars) and the RMSE for each PS model (grey bar). The best performance of the PS models has RF-LS 4 scored a maximum RMSE of 0.09 PI, which is close to the RMSE of 0.07 PI for the overall model. Increasing the LS to 36 results in an increased maximum RMSE of 0.8 PI for the PS models. The second ranking is for the ANN models (2x10 and 1x25) achieving a maximum RMSE of 0.33 PI and 0.43 PI. These are lower than the RMSE of 0.86 PI and 0.85 PI for the overall models.

Figure 8 shows that for LR, SVM, and ANN the PS RMSE values are smaller than overall RMSE values.

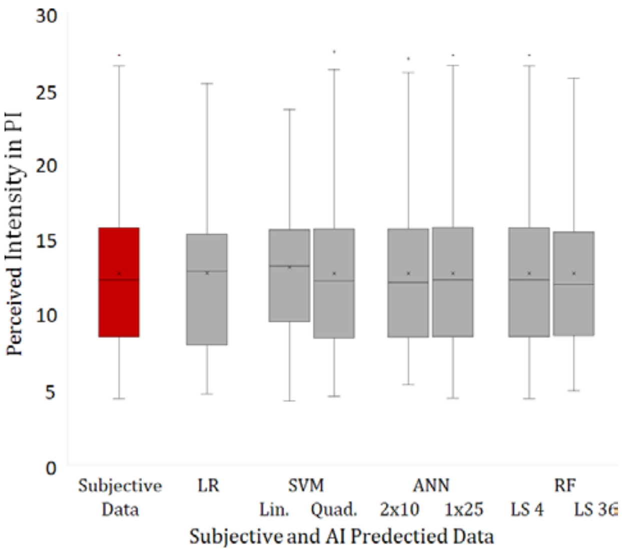

Figure 7. Distribution of subjective test data and prediction of the overall models.

For RF models the RMSE of overall model and PS models are more similar. The results indicate that the PS models should be used for their respective stores in the SC to predict PI rather than the overall model.

4. Conclusion

The results show the potential of VOC sensors for IAQ assessment in SC. Subjective and objective tests were conducted to validate the application of this technology with SC products. The use of AI models enables a correlation between the VOC-MGSS sensor signals and subjective values. To achieve this, an analysis of five AI models is conducted. The models were trained and tested with both overall and PS datasets. For model evaluation, RMSE metrics were applied. The best performance shows RF-approach-LS 4, achieving for the overall and SP dataset 0.07 PI and max. 0.09 PI. However, there may be an overfitting for this model [20]. For all model types except RF models, the results show a decreased RSME for product specific models compared to the overall models. The ANN models (2x10) and (1x25) achieved RMSE of 0.86 and 0.85 PI. This makes them also applicable for this dataset. Overall, further analyses with more subjective and objective data, especially validation data from field tests, are needed to bring such VOC-MGSS system into practice use. Moreover, a correlation of PI and acceptance, is needed for implementing these models in DCV concepts. ■

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References

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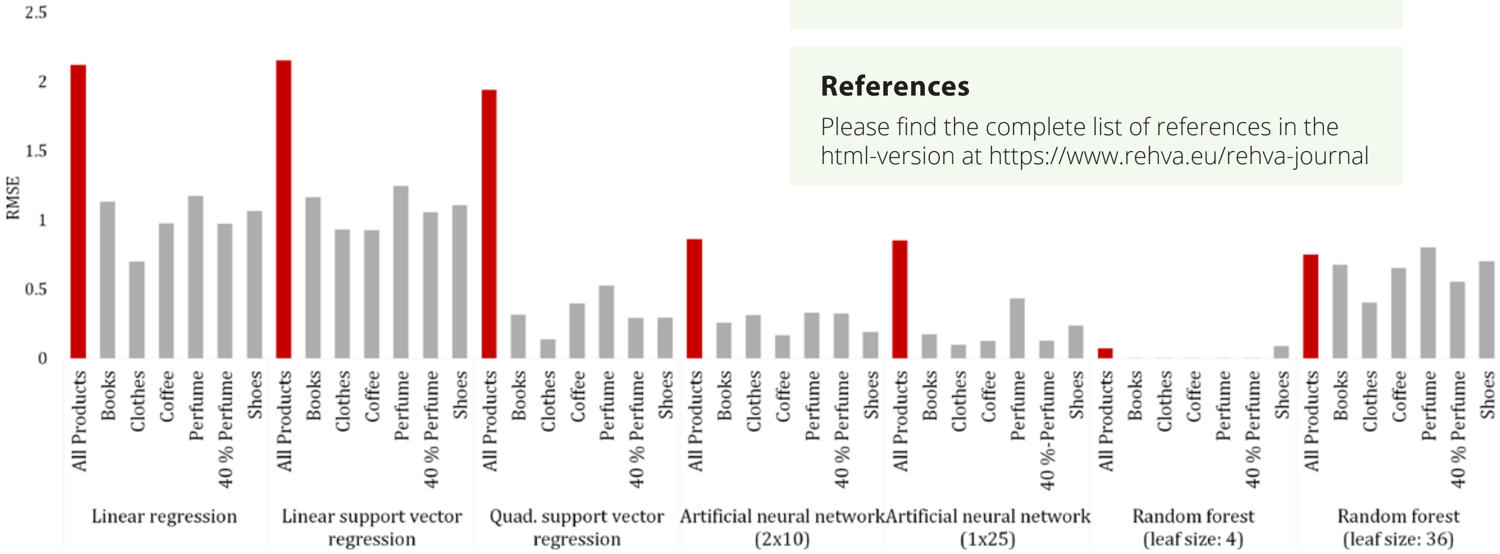

Figure 8. Comparison of the RMSE in PI for the overall and product specific models for testing.