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# The microwave gas sensors array driven by a decision tree algorithm for enhanced 3S parameters

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## Abstract

In the gas-sensing approach, 3S parameters are known as sensitivity, selectivity, and stability. The better the 3S parameters, the better the detection. Regardless of the detection nature of the gas sensors used to fabricate e-noses, the 3S parameters are universally used. In the case of microwave gas sensors, implementing e-noses is still pending. This paper presents the development of a decision tree algorithm to enhance the 3S parameters of microwave gas sensors based on metal oxides and tested under various conditions. A decision tree algorithm enables the detection of the *2n+2* gases. However, the theoretical analysis suggests that even more gases could be detected when the thickness of the gas-sensitive layer is optimized.

## 1. Introduction

The idea behind using electronic noses is to replace bulky, expensive reference analyzers such as gas chromatography-mass spectrometry (GC-MS) with easy-to-use, cheap, and portable systems [1, 2]. However, such replacement will affect the sensing process. In the gas-sensing community, 3S parameters [3, 4] (sensitivity, selectivity, and stability) are used to compare the various detection devices, including electronic noses. Regardless of the application of e-noses (e.g., air quality monitoring, air pollution detection, industrial processes where gases are produced in the reaction chain), the 3S parameters should be as high as possible. One method to increase the 3S parameters is to develop gas-sensing layers that detect several gases under various conditions. Another approach uses different transducers, such as microwave gas sensors (MGSs) instead of direct current (DC)-operated ones. Finally, utilizing machine learning (ML) and artificial intelligence (AI) algorithms paves the way for enhanced 3S parameter detection [5-8].

In this paper, a decision tree algorithm was applied to a microwave-based gas sensor array, and MGSs were tested under exposure to several gases used in air quality monitoring and industrial processes, including nitrogen dioxide ($NO_2$), acetone ($C_3H_6O$), ethanol ($C_2H_6O/C_2H_5OH$), isopropanol ($C_3H_8O$), methanol ($CH_3OH$), ethylbenzene ($C_8H_{10}$), propane ($C_3H_8$), ammonia ($NH_3$), and hydrogen sulfide ($H_2S$). Although MGSs have been intensively investigated for over a decade, the advent of e-noses based on MGS is still expected. One significant advantage of the MGSs is their ability to operate at room temperature. Moreover, the changes in the microwave measurement parameters pave the way for enhanced 3S parameters, allowing the development of e-noses capable of detecting gases in a mixture of compounds, where *2n+2* gases can be detected by *n* sensors only.

## 2. The concept of the decision tree algorithm

The decision tree algorithm (DTA) is a supervised learning algorithm commonly used in statistics, data mining, and machine learning algorithms (MLA) [9-10]; DTA is one of the most popular MLAs characterized by its intelligibility and simplicity. DTA is used as a predictive model and enables concluding a set of observations, in our case, about the impact of materials used for gas-sensitive layers deposition, applied measurement parameters such as operating temperature and frequency (ranging from kHz to THz). The concept of the DTA for the developed MGSs is given in Figures 1 and 2, where four (from all eight developed) interesting cases obtained in our study are presented and further discussed in section 3. The DTA is generally based on two sensors operating in different temperatures (room and medium temperature ~100ºC) and frequencies (kHz-THz). In each condition, the sensor could show no positive or negative response at low, medium, or high levels (more explanation in section 3). The trees have been separated, and it can be easily seen that each of the gases is detected using different parameters and sensor response characteristics.

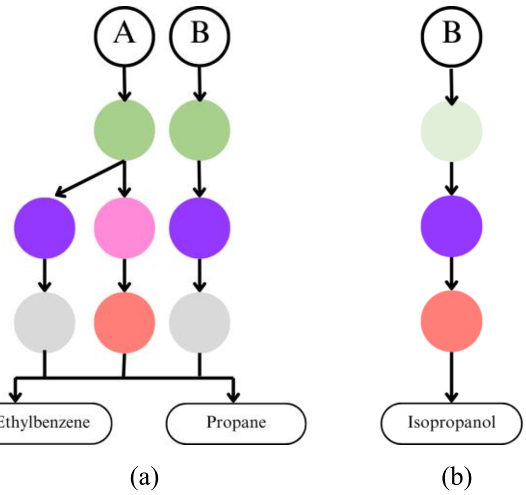
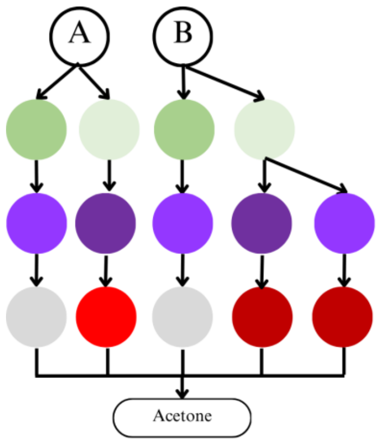



**Figure 1.** (a) The developed DTA to selective detection of ethylbenzene or propane; (b) isopropanol.

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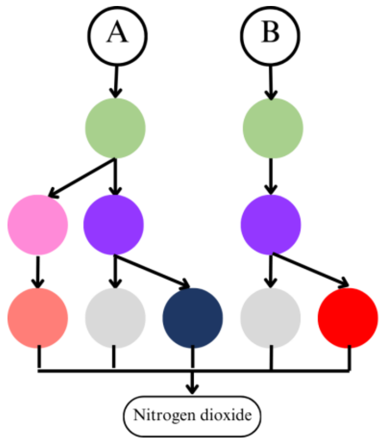
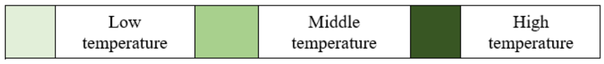



(d)

**Figure 2.** (a) The developed DTA to selective detection of acetone; (b) nitrogen dioxide.




(a)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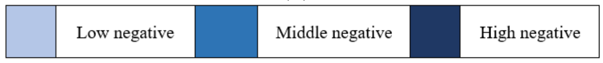


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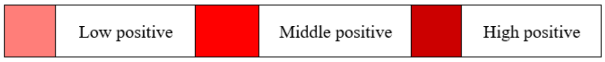


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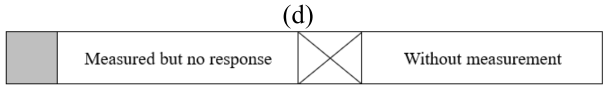


(e)

**Figure 3.** The legend for the colors used in the decision tree algorithms presented in Figures 1 and 2, (a) operating temperatures, (b) operating frequencies, (c) obtained negative responses, and (d) obtained positive responses (more explanation about MGS' sensor response in the main text), (e) no response or no measurement.

## 3. Results and discussion

The decision tree algorithms are tree-like structures used to make decisions based on a set of rules. Each node represents a question or condition, the branches correspond to possible answers, and the leaves contain the final decision or classification. The algorithm builds the tree from training data, selecting the most discriminating features to optimize decision accuracy. In the case of gas sensors based on the metal oxide gas-sensing layer (in this study: CuO and $SnO_2$) that works in a wide range of temperatures, eight gases can be effectively distinguished by analyzing sensor responses at different temperature and frequency conditions. Figure 3 shows the legend of colors used in Figures 1 and 2. As can be noticed, ethylbenzene and propane (Fig. 1a) exhibit identical responses under the given conditions, making them indistinguishable. On the other hand, isopropanol can be selectively detected using a specific set of parameters, as presented in Fig 1b. Two interesting cases are given in Figure 2. In the case of acetone, only positive responses (middle or high) can be obtained using various sets of parameters, including two gas-sensing layers used in this study. In contrast, the middle positive or high negative response can be found to detect nitrogen dioxide.

The presented data suggest that analysis of the signals without knowledge about the initial gas composition is not trivial, and neural networks (NN) should be considered for enhanced detection. However, for effective use of various NNs such as Convolutional neural networks (CNNs), Recurrent neural networks (RNNs), Radial basis function (RBF), Long short-term memory (LSTM), Multilayer perceptron (MLPs), Generative adversarial networks (GANs) [11-15] more sophisticated measurement scenarios have to be conducted, what was out of scope of this study. Contrary to typical resistance or conductance changes of DC-operated gas sensors based on metal oxide gas-sensing layers, microwave gas sensors can operate in resonant frequency shift and wideband measurements [17]. Both methods have advantages and disadvantages; therefore, deciding a priori which method should be applied is impossible. The cost of the measurement setup components, the knowledge about the signal analysis, and the scalability of the fabrication of microwave gas sensors, including microwave circuits that work as signal transducers and gas-sensing layers, should be considered. In our research group, wideband measurements are preferred, as reported previously [17-18]. In this study, the electronic nose was equipped with six gas sensors. The concept of the e-nose was previously presented and described [19]. Briefly, it contains typical components such as the gas-sensing chamber (all sensors are placed and tested under the same conditions) equipped with gas-dosing lines that offer various conditions, e.g., relative humidity changes (RH%) and temperature (T). The e-nose is fitted with heaters that provide separate heating for each sensor placed in the chamber. Thus, the sensors can be tested at various configurations; however, if one sensor works at 200°C, another will also be heated. Therefore, the testing procedure should start at room temperature and then go up to operating temperatures.

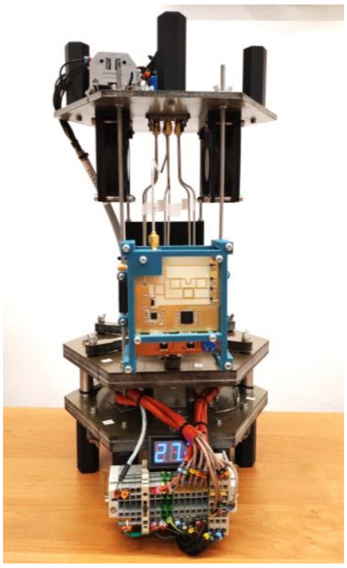

**Figure 4.** The first plan presents a photograph of the electronic nose measurement device developed in the project for microwave gas sensors with a dedicated microwave measurement circuit.

The microwave circuits used as gas sensor substrates have been previously presented in detail in [17, 18]; however, in Figure 4 on the first plane, the dedicated microwave measurement circuit (MMC) is well presented. MMC is based on the 8-port reflectometer concept where 4-quadrature couples and 2 in-phase power dividers were designed. The calibration and measurement protocol was elaborated in detail in [17]. However, a significant element of the entire device is a mechanical switch (CCR-38S360 from Teledyne Relays) that enables switching between sensors to capture the signals. A single MMC can support up to six sensors in such an approach. However, all mechanical switches are characterized by a finite number of switches that can be done, and this should be taken into account when the e-nose device is planned for research and development as well as fabrication and production. An innovative approach to reduce the number of switches and, in turn, enhance the long-term operation of e-nose before switch replacement is using a measurement protocol where sensors are measured only at specific time points to calculate the gas sensor responses, as illustrated in Fig. 5.
Every sensor in the chamber is tested at least once in the continue mode to check the response curves (response nature of the sensor) and further only shortly before and after the introduction of gases into the gas-sensing chamber to measure the sensor response signal that can be defined as a change of resistance, conductance, impedance or as in our case the change of phase of microwave gas sensors. Therefore, the gas sensor response ($S$) is calculated as $S$=$\varphi_{gas}$-$\varphi_{air}$, where $\varphi_{gas}$ and $\varphi_{air}$ represent the phase values under exposure to target gas and synthetic air (or ambient air), respectively.

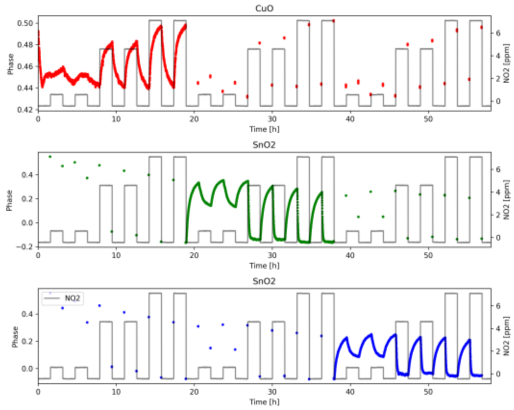


**Figure 5.** The MGS responses

In summary, the microwave gas sensors array driven by a decision tree algorithm for enhanced 3S parameters can be achieved, as presented in this paper. Regardless of the gas-sensing detection method used in the device, the principles of the DTA are the same and, therefore, can help researchers to define several parameters, such as: (**i**) what kind of gas-sensing materials should be used. Even if we have limited our study to metal oxide-based material, we decided to verify p-type (CuO) and n-type ($SnO_2$) semiconductors. However, other gas-sensing materials for MGSs have also been tested [20] and could be included in DTA; (**ii**) choose an operating temperature that enables the detection of a specific gas compound in the gas mixture. Figures 1 and 2 show that the same material at the same frequency but at various operating temperatures may exhibit sensitivity to other molecules and vice versa (**iii**) choose an operating frequency. As was mentioned above, two additional modes of working (resonant and wideband) can be added to the DTA; (**iv**) the number of sensors can also be included in the DTA. However, this issue is limited to technical limitations of the developed gas sensor chamber in the electric nose; although the number of sensors has an impact on the number of gases that can be detected according to the 2n+2 formula, in practice sometimes is easier and cheaper to use independent chambers instead of a single one as was done in this study; (**v**) the material's properties such as oxidation state, stichometry vs. non-stichometry, thickness, form (nanostructures vs. bulky) also is essential.

## 4. Conclusions

This study underscores the importance of utilizing multiple frequencies and temperature conditions in gas detection systems to improve accuracy and differentiation among gases. The classification framework proposed in this paper provides a structured approach to gas identification, which can be further refined with additional sensor parameters and environmental conditions.

## 5. Acknowledgements

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