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Sniffing Smartwatch for Online Monitoring of Selected Odorants

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Monitoring chemical substances is of paramount importance in various industries and environmental contexts. In industrial settings, the presence of certain chemical substances may indicate leaks, spills, or malfunctioning equipment, posing immediate threats to both human health and the environment. Moreover, continuous monitoring of chemical compounds is crucial for ensuring compliance with safety regulations and environmental standards. In the context of air quality management, monitoring chemical compounds helps identify sources of pollution, assess the impact on public health, and implement effective pollution control measures. Timely detection and response to chemical compounds also play a vital role in preventing long-term environmental degradation. Overall, monitoring chemical substances is an indispensable component of proactive risk management, environmental stewardship, and the safeguarding of human well-being. The development of automatic and portable devices for online monitoring is an important need in the chemical industry. The smartwatch designed and presented is a home-developed prototype and built from commercially available components. All components of the smartwatch are protected with a plastic casing capable of allowing air to pass to the sensors, the device is also capable of measuring temperature and relative humidity, magnitudes that influence the detection of different odors or volatile compounds. This device is based on a microcontroller that offers low-power performance, integrated Bluetooth low energy at an affordable price, and the measurements of four digital MOX gas sensors, models BME680 SGP40, ENS160 and STC31 through I2C interface. Data are shown on a LCD display and also transmitted via Bluetooth to a smartphone at a sampling period time of 2 s. It is powered using a 3.7 V lithium polymer battery. The smartwatch has a graphical interface to show the user the data provided by the sensors. The designed smartwatch has been validated by measuring different industrial gases like toluene, xylene, and ethylbenzene at low concentrations. Toluene was measured at 6 ppm, xylene at 8 ppm, and ethylbenzene at 10 ppm. Good discrimination between the three different gases was achieved using Principal Component Analysis as multivariable analysis.

* 1. Introduction

In recent years, ambient air quality has been an important topic related to human health. Air pollution has been related to respiratory diseases, and cardiovascular diseases among others as it was collected in the work made by (Almetwally et al., 2020). Some chemical agents like toluene, xylene, and ethylbenzene are points of interest as they are used in different industrial processes (Jingjing et al., 2021). The work made by (Chaiklieng, 2021) shows that exposure to xylene and ethylbenzene is related to abnormal and neurological effects. Furthermore, (Cruz et al., (2014) showed that toluene exposure produces motor incoordination, dizziness, relation, and lightheadedness. Reference values of exposure limits to these gases can be found in the occupational exposure limits made by the Spanish Ministry of Work (LEP, 2024). According to this guideline, toluene and xylene exposure limits in an 8-hour labor day must not exceed 50 ppm and ethylbenzene must not exceed 100 ppm.

Normally air quality measurement systems are found in fixed and few locations because of their price, which implies that measurements are made in single locations and sometimes are not a reliable representation of the environment. For that reason, there is a need for cheaper and portable devices that can measure air quality, an alternative to conventional air quality stations are electronic noses. Electronic noses are devices capable of measuring different chemical substances. Electronic noses, also called e-noses are formed by the combination of different gas sensors that transform an odor into an electrical signal and a pattern recognition system (Di Pizio et al., 2020). The different types of sensors used in electronic noses are optical, surface acoustic wave, electrochemical, catalytic, and semiconductor. The most commonly used are semiconductor-based sensors, also called metal oxide semiconductors (MOX). The advantages of MOX sensors are the ability to detect a wide range of gaseous chemical compounds and miniaturization capabilities. However, they present low sensitivity and low selectivity, and their response is affected by different environmental factors (Park et al., 2019).

Different works have used personal devices to measure air quality based on electronic noses. (Dhingra et al., 2019) developed a system based on the Arduino platform to monitor air pollution using a CO, CH4 and an Air quality gas sensor, data from the sensors were sent to a cloud. (Arroyo et al., 2019) designed a wireless portable e-nose that used 4 different MOX sensors to detect different concentrations of NOx.The work made by (Palomeque-Mangut et al., 2022) proposed a personal device conformed by MOX sensors that mapped the surrounding air quality.

This work presents a novel portable electronic nose integrated into a smartwatch, the electronic nose designed includes MOX sensors and also a temperature/humidity and an accelerometer sensor, the device can communicate via Bluetooth Low Energy (BLE) to a smartphone to monitor air quality in real-time. The main advantage of this device is the inclusion of gas sensors in a smartwatch to detect air pollutants, for that reason the device is optimal for users to monitor the surrounding air quality. To validate the device, measurements with industrial gases like toluene, ethylbenzene, and xylene are made to test the discrimination capabilities of the device.

* 1. Materials and Methods
		1. Description of the SmartWatch

The Smartwatch designed whose block diagram is shown in Figure 1a, is composed of 4 different MOX sensors to improve the detection capabilities of the device, an accelerometer, and temperature/humidity sensors. The sensors send data from the gases detected to a microcontroller, the microcontroller also sends data via Bluetooth to a Smartphone and shows the data from the sensors to a LDC screen. The power supply is provided by a Lithium polymer battery and the smartwatch is charged by a wireless charger. The device’s case is also shown in Figure 1b, which allows a continuous airflow inside of it for the measurement of air compounds.

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*Figure 1. Block diagram of the Smartwatch designed (a). Smartwatch developed (b).*

4 different MOX commercial sensors are included in the electronic nose, they communicate via I2C to the microcontroller, different sensors are used to provide different information that allows to improve the detection capabilities of the target gases. The sensors used and their respective data measured are the following:

* ASM330LHH from STMicroelectronics: accelerometer and gyroscope sensor.
* BME680 from Boch: MOX sensor that gives values from temperature, relative humidity, pressure, and resistive values.
* SGP40 from Sensiron: MOX sensor that provides raw resistive values.
* ENS160 from ScioSense: MOX sensor capable of measuring information from raw resistance signals, total volatile organic compounds(TVOCs), equivalent CO2 from volatile compounds, and Air Quality Index (AQI) values based on TVOCs signal.
* STC31 from Sensirion: MOX sensor, measures CO2 vol % in air based on thermal conductivity.
* SHT40 from Sensiron: digital temperature and relative humidity sensor

The Microcontroller used is a 32-bit STM32WB55 from STMicroelectronics. This microcontroller includes internally a dedicated Bluetooth Low Energy 5.0 Core, which is used to send data information from the sensors to a Smartwatch, the smartwatch is configured to send data from the sensors every 2 seconds. In addition, the microcontroller communicates via SPI with a LCD screen. The main screen is shown in Figure 2, it shows the time information and also information from the sensors. The relative humidity and temperature measurements of the environment are provided by the SHT40. In addition, the atmospheric pressure was measured by the BME680. TVOCs, equivalent CO2, and AQI from ENS160 are also shown. The AQI values depend on the values of TVOCs, there are five different levels, which are explained in Table 1. AQI values are represented with circle colors to show qualitatively the measurements so that the device can be used with nonexperienced users.



*Figure 2. Main menu of the SmartWatch.*

*Table 1: AQI limits from ENS160 and their meaning.*

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| AQI  | Color | Hygienic Rating | Exposure Limit |
| 5 | Red | Situation not acceptable | hours |
| 4 | Orange | Major objections | <1 month |
| 3 | Yellow | Some objections | <12 months |
| 2 | Green | No relevant objections | No limit |
| 1 | Blue | No objections | No limit |

The SmartWatch is powered by a Lithium polymer battery at 3,7 V. The battery is charged via the LTC4124 battery charger circuit, this circuit allows to charge the battery wirelessly via transmission and receiver coils and also by a DC source. The voltage from the battery is converted to +3.3 Vdc via a Buck-Boost converter to supply the microcontroller and the sensors (SHT40, BME680, SGP40, STC31, and ASM330LHH). Furthermore, a +1.8 V voltage regulator is used to reduce the voltage to power the ENS160 sensor.

* + 1. Experimental setup

The experiment performed to test the detection capabilities of the device was made with a gas generator (OVG-4 from Owlstone) and a humidity generator to adjust the concentration of three different gases toluene, ethylbenzene, and xylene, additionally, permeation tubes of each gas were used as a sample source.

Toluene was measured at 6 ppm, xylene at 8 ppm, and ethylbenzene at 10 ppm, the concentration values measured were taken below the limits explained in Section 1 to test if the device could detect lower concentrations. 10 repetitions were made at each gas concentration and the measurement time was 4 minutes for sample gas (absorption) and 8 minutes for reference air (desorption), the sampling time was 2 seconds and the relative humidity selected was 40 %.

Permeation Tubes were introduced in the gas generator, and the desired concentration of each gas was achieved by changing the temperature of an oven integrated into it, temperatures programmed to reach the target concentrations explained above for toluene, xylene, and ethylbenzene are respectively 61, 81, and 95ºC, according to Eq(1), were C is the concentration (ppm), qd is the permeation rate, M is the molar weight of the gas and Q is the total flow ( sample flow+humidity flow) which value was adjusted at 150 ml/min.

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| $$C=\frac{24,45∙q\_{d}}{M∙Q}$$ | (1) |

The experimental setup is shown in Figure 3. Dry air passes through both the humidity generator and the gas generator after that, the mixture of wet air and sample air passes through the smartwatch that was located in a methacrylate cell to ensure a uniform flow through the sensors. Finally, data is sampled every 2 seconds and sent to a smartphone via Bluetooth for future analysis.



*Figure 3. Experimental setup.*

* 1. Results and discussion

Figure 4 shows the response of ENS160’s volatile signal when toluene at 6 ppm, xylene at 8 ppm, and ethylbenzene at 10 ppm is measured, it can be observed that the sensor can detect the target concentration of the gases and the shape of the signals measured are different so, a clear different response to the gases can be seen, in addition, the 10 repetitions performed on each gas are similar as concentrations are constant.

To reduce the dimensionality of the data and classify the gases principal component analysis (PCA) was used on the 10 repetitions made. All the data from all the sensors were taken except the relative humidity and temperature variables as they remained constant in the experiment. In addition, the first repetition of each gas was deleted to reduce the dispersion. Figure 5 shows the PCA obtained, it shows a clear dispersion and classification between each gas group and the total variance explained between the two principal components is 81%.



*Figure 4. Response of ENS160 to 6 ppm Toluene (above), response of ENS160 to 8 ppm Xylene (middle), response of ENS160 to 10 ppm Ethylbenzene (below).*



*Figure 5. 2-D Principal component analysis of the 3 gases measured.*

* 1. Conclusions

A novel portable electronic nose integrated into a Smartwatch has been developed, the electronic nose integrates different MOX sensors to improve the discrimination capabilities.

 The device has been tested with different gases used in industrial processes like toluene, xylene, and ethylbenzene. The concentrations generated for each gas were respectively 6 ppm, 8 ppm, and 10 ppm. These values are lower than the listed in legislation cited in Section 1 being the limit values for Toluene 50 ppm, Xylene, 50 ppm, and Ethylbenzene, 100 ppm.

Principal component analysis was used as multivariable analysis and for dimensionality reduction. The results showed that the device can detect and discriminate the gases measured at low concentrations. For that reason, the device has proved that can be used by users to detect leakages at lower concentrations than legislation limits.

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References

Almetwally, A.A., Bin-Jumah, M., Allam, A.A., 2020. Ambient air pollution and its influence on human health and welfare: an overview. Environmental Science and Pollution Research. https://doi.org/10.1007/s11356-020-09042-2

Arroyo, P., Herrero, J.L., Suárez, J.I., Lozano, J., 2019. Wireless sensor network combined with cloud computing for air quality monitoring. Sensors (Switzerland) 19. https://doi.org/10.3390/s19030691

Chaiklieng, S., 2021. Risk assessment of workers’ exposure to BTEX and hazardous area classification at gasoline stations. PLoS One 16. https://doi.org/10.1371/journal.pone.0249913

Cruz, S.L., Rivera-García, M.T., Woodward, J.J., 2014. Review of Toluene Actions: Clinical Evidence, Animal Studies, and Molecular Targets. J Drug Alcohol Res 3, 1–8. https://doi.org/10.4303/jdar/235840

Dhingra, S., Madda, R.B., Gandomi, A.H., Patan, R., Daneshmand, M., 2019. Internet of things mobile-air pollution monitoring system (IoT-Mobair). IEEE Internet Things J 6, 5577–5584. https://doi.org/10.1109/JIOT.2019.2903821

Di Pizio, A., Behr, J., Krautwurst, D., 2020. Toward the Digitalization of Olfaction, in: The Senses: A Comprehensive Reference. Elsevier, pp. 758–768. https://doi.org/10.1016/B978-0-12-809324-5.24147-3

Jingjing, Z., Zhanwu, N., Weijie, L., Peng, Z., Jinhua, L., Yanni, Z., Ning, L., Yiting, J., Peng, S., 2021. High-sensitive metal oxide gas sensor for BTEX gases based on ternary composite of Ce xMn1-xO2/SnO2. Meas Sci Technol 32. https://doi.org/10.1088/1361-6501/ac14f4

Límites de exposición profesional para agentes químicos en España. 2024, n.d.

Palomeque-Mangut, S., Meléndez, F., Gómez-Suárez, J., Frutos-Puerto, S., Arroyo, P., Pinilla-Gil, E., Lozano, J., 2022. Wearable system for outdoor air quality monitoring in a WSN with cloud computing: Design, validation and deployment. Chemosphere 307. https://doi.org/10.1016/j.chemosphere.2022.135948

Park, S.Y., Kim, Y., Kim, T., Eom, T.H., Kim, S.Y., Jang, H.W., 2019. Chemoresistive materials for electronic nose: Progress, perspectives, and challenges. InfoMat. https://doi.org/10.1002/inf2.12029