DOI 10.5162/SMSI2025/C3.4

Towards Low-Cost Portable GC Systems for VOC Analysis

Omar Tarek Penagos Carrascal[1,2], *Maximilian Köhne*[1,2], *Gina Zeh*[1], *Tilman Sauerwald*[1,2]
[1] *Fraunhofer Institute for Process Engineering and Packaging IVV, Department of Sensory Analytics and Technologies, Giggenhauser Strasse 35, 85354, Freising, Germany*
[2] *Saarland University, Campus A5.1, 66123 Saarbrücken, Germany*
omar.tarek.penagos.carrascal@ivv.fraunhofer.de

Summary:

A gas chromatography system with a metal oxide semiconductor gas sensor as detector was designed, built, and tested for the detection of hexanal, octanal, and acetic acid. The system consisted of a manual sample injection using a gas-tight syringe (100 µL) and with helium as carrier gas. A free fatty acid phase column (L: 15 m ID: 0.25 mm, coating: 0.25 µm), kept in an oven at 80°C, promoted the selectivity of the sensor via gas separation. The sensor used for detection was a Sensirion SGP40, whose four sensing layers were operated isothermally at 300°C. The system was able to measure the presence of individual compounds based on their retention times, specifically hexanal (RT ~70 s), octanal (RT: ~160 s) and acetic acid (RT: ~470 s). Sharp detector peaks were achieved from the first derivative of the sensor signal.

Keywords: Gas chromatography, VOC analysis, phase equilibrium, MOS sensor, system optimization

Introduction

Reducing the size and cost of gas chromatographs (GCs) to portable versions is a challenging task due to their high complexity. Traditional GCs incorporate expensive components to handle a wide range of applications and measure a broad range of substances. To make GCs portable and affordable, one strategy is to narrow the focus to specific applications. By doing so, it becomes possible to replace high-cost components with more affordable alternatives that can still provide adequate results for those specific scenarios.

The main objective of the current study is to conceptualize and demonstrate the feasibility of a portable GC comprising inexpensive components. The field of application is the measurement of volatile organic compounds (VOCs) for the analysis of polymer recyclates and olive oil.

For this purpose, it is necessary not only to build the device, but also to optimize its configuration by means of mathematical models that describe the phase equilibrium along the device, as well as to optimize the sensor system operation and data analysis. A practical approach to achieving this is to evaluate each stage of the GC process independently: Injection/sampling, separation, and detection [1]. This abstraction provides a clearer view of which parts can be simplified or replaced.

In VOC detection, a metal-oxide-semiconductor (MOS) sensor can be used as a lower-cost alternative to more complex detectors [2]. In applications where analyte concentrations are too low for detection, the use of a preconcentrator may be necessary to increase system sensitivity and maintain a reliable detection. This means that a sampling/injection system must be designed and optimized to achieve the highest preconcentration of the substance to be analyzed.

The separation takes place inside a GC column coated with a stationary phase that interacts with the different components in the sample. The difference between these interactions causes the compounds to flow at different rates through the column, resulting in separation. The challenge is to achieve a separation good enough to detect the substances of interest while keeping costs low (a GC column as short as possible and a suitable temperature program).

In this work, we present a demonstrator for the simultaneous detection of selected volatiles.

Materials and results

Helium is used as carrier gas and is introduced into the system through a mass flow controller (MFC) at a constant rate of 3 mL/min. Injection into the system was performed manually using a Hamilton gas-tight syringe, introducing a total sample gas volume of 100 µL. The syringe was used to take a headspace sample from a vial containing a mixture of the target substances. The following substances were chosen for a first qualitative test of the system: acetic acid, octanal

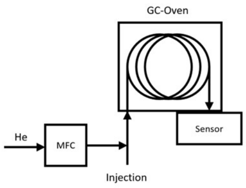

Figure 1: Process flow diagram of the system

Figure 2: Interior (left) and exterior casing (right) of the system

and hexanal, which are all typical odorants in recyclates [3].

An oven was built containing a 40 W 24 VDC heating element from Triangle Labs. The temperature controller was a Wachendorff UR43838. An Agilent HP-FFAP GC column (L: 15 m ID: 0.25 mm, coating: 0.25 µm) was installed and a sensor array SGP40 from Sensirion was connected at its outlet. The sensor system has four sensing layers, each of which deliver a signal. All sensor layers were held at 300 °C and the oven was operated isothermally (80 °C). The system was controlled by a Siemens PLC through Python using the snap7 package (see Figure 1 and Figure 2).

Figure 3 (left side) shows the signals emitted by the sensor system, with S being defined as the subtraction of the raw value from the maximum possible raw value ($S = 65535 - R$).

All four layers of the sensor show three maxima, showing that separation of the odorants within the gas mixture was successful, and the chosen sensor was able to detect the substances at the chosen concentrations. Tests with each of the substances individually confirmed that the peaks corresponded to hexanal, octanal, and acetic acid, respectively. Some peaks overlap (e.g., first sensor layer, red curve), which can make it difficult to measure the substances quantitatively or even to distinguish them. To overcome this issue, a first derivative analysis is performed on the sensor signal. For this, the curve was smoothed using the *gaussian_filter1d* function from the *SciPy* package for Python. The first derivative is shown in Figure 3 (right side).

Outlook

The developed system was able to separate the three selected substances. Further optimization and development work is currently in progress, including the design and optimization of a preconcentration/injection system to replace the manual injection, optimization of the detection stage, and evaluation with other analytes.

References

[1] M. Köhne, G. Zeh, C. Schmidt, and T. Sauerwald, “P13.4 - Entwicklung eines kostengünstigen Gaschromatographie-Systems für die Messung von Reifegas mit Kompensation der Temperatureinflüsse auf die Säule,” in *Poster*, Online: AMA Service GmbH, Von-Münchhausen-Str. 49, 31515 Wunstorf, Germany, 2021, pp. 338–342. doi: 10.5162/15dss2021/P13.4.

[2] A. Schütze *et al.*, “Highly Sensitive and Selective VOC Sensor Systems Based on Semiconductor Gas Sensors: How to?,” in *Environments*, Mar. 2017, p. 20. doi: 10.3390/environments4010020.

[3] M. Strangl, E. Ortner, T. Fell, T. Ginzinger, and A. Buettner, “Odor characterization along the recycling process of post-consumer plastic film fractions,” *Journal of Cleaner Production*, vol. 260, p. 121104, Jul. 2020, doi: 10.1016/j.jclepro.2020.121104.

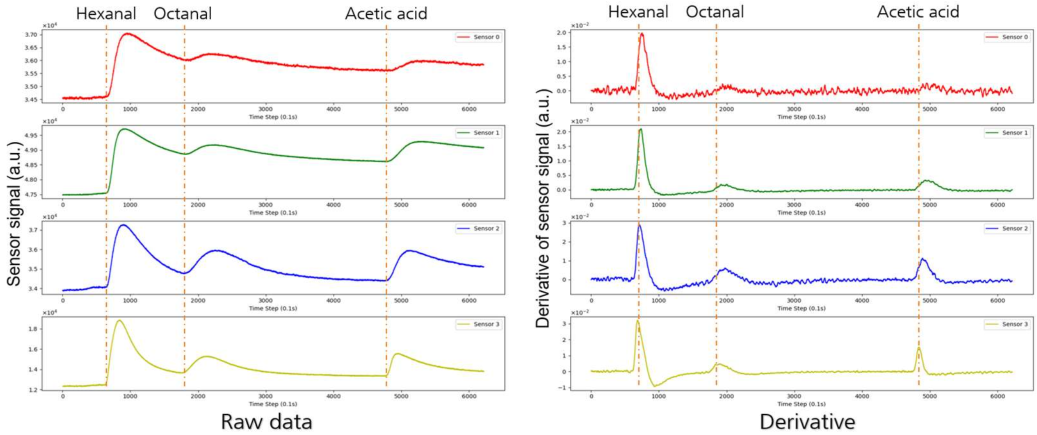

Figure 3: Measurement results, raw data (left) and derivative (right)