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► **To cite this version:**

Pedro C. Moura, Valentina Vassilenko, Jorge M. Fernandes, Paulo H. Santos. Indoor and Outdoor Air Profiling with GC-IMS. 11th Doctoral Conference on Computing, Electrical and Industrial Systems (DoCEIS), Jul 2020, Costa de Caparica, Portugal. pp.437-444, 10.1007/978-3-030-45124-0_43 . hal-03741570

HAL Id: hal-03741570

<https://inria.hal.science/hal-03741570v1>

Submitted on 1 Aug 2022

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Indoor & Outdoor Air Profiling with GC-IMS

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Abstract. Air Quality research is a trending topic that has received increasing attention from scientific community around the globe. Due to the high relevance of recent discoveries in areas like medicine or chemistry, analytical techniques with high sensitivity and selectivity play a crucial role in the characterization of the ambient air composition. This preliminary study intends to evaluate the air quality around a university campus by profiling VOCs from 14 locations with differentiated characteristics, intended for further industrial contextualization. Multiple air samples were collected from each defined location and further analysed with the GC-IMS technique. Totally, 33 compounds were detected, and their intensity peak values, and drift and retention times were used to identify 11 of them. The suitability of GC-IMS to quickly and easily assess air quality become evident. Further detailed studies should include a wider range of locations to identify new VOCs and their eventual consequences to human health.

Keywords: Gas Chromatography, Ion Mobility Spectrometry, Air Quality, Intensity Profiling, Volatile Organic Compounds.

1. Introduction

Volatile Organic Compounds as aromatic hydrocarbons, aliphatic, aldehydes, ketones, ethers, acids and alcohols, are inert compounds with the capability of passing through biological membranes and, according to its concentration, may be harmful to human health [1]. The increasing health problems related with the chemical composition of environmental air requires a careful and detailed study on the identification and quantification of these compounds in air samples and possible consequences to human health [1]. Being mainly released to the air from different sources, such as building materials, furniture, cleaning and preservation products, and activities-related materials, the study of Volatile Organic Compounds is crucial both for indoor and outdoor air quality assessment [2]. Although IMS spectra information of several VOCs is still unknown (e.g., Toluene, Xylenes and Ethylbenzene), [3], [4], there are some well-known VOCs that are characteristics of environmental air samples, like Ethanol,

Acetone, Ethyl Acetate and 2-Propanol [5] Common compounds such as Ammonia or Isoprene, for example, are characteristics of human breath [6]. The continuous exposure to possibly noxious and hazardous compounds, thus revealing the importance of air quality studies which should include VOCs monitoring and their quantification, at the workplace, home, schools and other public places [2], [7], [8], [9].

Nowadays, several techniques are used to assure the air quality of samples from several locations and matrixes [10].

GC-IMS is an analytical technique that was initially developed for use in military context, specially to detect explosive and chemical warfare agents [11], [12]. Recently, it gained a new role in several civil applications such as the detection of a wide range of analytes, for health, security or even food or air quality purposes [13], [14]. The wide range of applications is due to the technique advantages because it combines the best characteristics of both GC and IMS. GC is known for its good precision, wide dynamic concentration range and high selectivity and sensitivity [15], [16]. IMS, on its turn, is a highly sensible technique that allows good analytical flexibility and real time monitoring at a low cost [17]. Coupled in a single device, GC-IMS technique offers improved quality at differentiating organic compounds by its size, weight and shape when compared with other techniques [17], [18].

The functional principle of GC-IMS is easily and widely understood. A sample is injected into the apparatus and it will undergo pre-separation by Gas Chromatography in which the compounds are separated into individual components [19]. The time compounds take to elude from the GC column is called Retention Time (RT) [15], [17]. Compounds are, then, transported into the IMS, where they are ionized by a radiation source. After the ionization, the formed ions are exposed to a weak and homogeneous electric field that moves each molecule across a drift tube. The time that the ions take to go through the drift tube is called Drift Time (DT). The ions are, then, separated according with their specific ion mobilities thus arriving at different times at the detector, also known as Faraday Plate [20]. After the entire process, a three-dimensional spectrum is produced in which the drift time, the retention time and the intensity are represented. Intensity, normally, is represented by a colour scale and corresponds to the sample concentration of each compound [21].

2. Contributions to Life Improvement

As mentioned before, the characteristics and composition of the environmental air, the presence or absence of certain compounds and its concentrations/intensities have direct effects on population's health. The mapping, detection and quantification of these volatile organic compounds are very important parameters that should be studied. The study developed in this article intends to study the air quality around a university campus to prove the suitability of GC-IMS to identify and quantify distinct volatile organic compounds in different air samples. The obtained results are intended to demonstrate the eventual necessity of taking necessary measures about human exposure to possibly noxious compounds. Better knowledge about different locations profile will allow to protect human beings and prevent eventual health problems that may appear due to the presence of harmful compounds.

3. Materials and Methods

3.1 Chosen Locations to Collect Air Samples

To characterize the university campus air, fifteen locations were chosen based on its characteristics (i.e., specific smells, presence of different machines, use of distinct chemical products or big affluence of people). From these fifteen locations, one of them was used as reference air and the remaining fourteen were comparatively analysed against the reference. The ambient air present in the laboratory where the GC-IMS apparatus is located was selected as reference, and the other fourteen selected locations were mostly facilities where some specific VOCs are supposed to vary its production levels. Locations where air samples were collected are GC-IMS Laboratory (Reference Air), Electronics Laboratory, Chemistry Laboratory, Administration Building Entrance, Conservation and Restoration Laboratory, Atomic and Molecular Physics Laboratory, Biomechanics and Hemodynamic Laboratory, Electronic Engineering Building, Mechanical Engineering Building, FABLAB – Fabrication Laboratory, Canteen, Materials Engineering Laboratory, Bathroom, Parking Lot, Workshop.

3.2 Air Collection Method

A chemically inert manual Teflon pump with an accoupled stopcock valve was used to collect and isolate the air samples from the different locations. Such procedure allowed to obtain contamination-free gaseous-phase air samples, avoiding the interaction and influence of exogenous compounds. This way, location-characteristics samples were able to be transported for characterization with the GC-IMS.

3.3 GC-IMS

The GC column used was an MXT-200 with 30 m length and 0,53 mm internal diameter coated with stainless steel with a mid-polar stationary phase of trifluoropropylmethyl polysiloxane with a thickness of 1 μm . The IMS instrumentation used was a BreathSpec® device from GAS Dortmund equipped with a Tritium H^3 (β -radiation) 300 MBq as an ionisation source. The drift tube has a 5-kV switchable polarity and a tube length of 98 mm with an electric field strength of 500 V/cm.

Air samples analysis was performed through its injection into the GC-IMS apparatus by compressing the plunger of the pump system for approximately 3 seconds. The above-mentioned procedure was repeated three times for each location to minimize the effects of potential contaminant compounds and losses of environmental airs' specific compounds. Every single analysis performed in GC-IMS produced a three-dimensional spectrum (fig. 1). All obtained

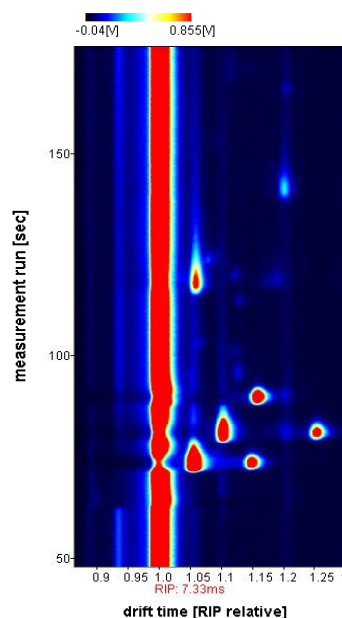


Fig. 1. Example of a spectrum produced by the GC-IMS technique.

spectra were analysed and compared with LAV software (G.A.S. Dortmund) and the values of intensity, drift time and retention time of all signals were collected.

The variation of each maximum relative intensity values (intensity peaks) among all spectra allowed to plot a characteristic graph of compounds for each studied location. Such graphs represent the relative intensity of each compounds in the labelled location. The presented intensity values are relative to the values in the reference air, i.e., a value of zero in the *y*-axis indicates a similarity in the concentration of that compound when comparing both locations. As relative intensity values, a bar that appears above the referential indicates a higher concentration of that compound relatively to the reference air. To provide a better understanding of the profiles, all the charts have the same *yy* values (3.5), the bars that exceed this value are labelled with the corresponding value. A radar graph was also plotted coupled to the bars charts to ease the profile visualisation. Additionally, both drift and retention times allowed the identification of some of the found compounds using pre-developed libraries.

4. Results and Discussion

Overall, fourteen locations were studied and compared relatively to a fifteenth. The choice of GC-IMS apparatus laboratory as reference air is due to the deep knowledge authors already have about its composition. The choice of another air as reference would imply a change in the obtained profiles (further studies will have this topic in consideration). Three samples were done for all locations totalizing 45 spectra. In total, 33 VOCs were found and 11 were identified. Relative intensity values (bars) and intensity profile (line) for four locations are represented in figures 2 a) - d). For the remaining locations, only the radar chart is represented (fig. 3 a) - i)), still allowing visual comparison among the different campus locations. Table 1 (appendix) lists all 11 drift and retention times for the identified compounds and their CAS numbers. Some of those identified compounds are dimers and trimers of a same compound. There are no new or extinguished compounds from place to place, however, their peak intensities vary considerably across locations.

Most of the compounds present in the air of Electronics Laboratory (fig. 2 a)), of Chemistry Laboratory (fig. 2 b)), and of Biomechanics and Hemodynamic Laboratory (fig. 3 c)) have higher intensities relatively to the reference air. All three locations even contain two compounds which concentrations are much higher than the remaining, respectively, compound 8 (2-propanol) and 21 (unidentified) to the first location, 17 (unidentified) and 21 to the second, and 8 and 21 to the third. Compound 21 is also very intense in some other locations what proves its possible relation with the activities done in the location. There are other locations, such as the Electronic Engineering Building (fig. 2 d)) and the Conservation and Restoration Laboratory (fig. 2 c)), where the compounds intensity is lower when compared to the reference air. On its turn, the intensity profile for the Physics Laboratory (fig. 3 b)) shows the VOCs concentration it is generally the same of the reference air. The compound Ethyl-acetate (bars 8 and 33) has similar concentrations across the different locations but in the Workshop (fig. 3 i)) its intensity increases considerably which indicates that this location has some ethyl-acetate production source.

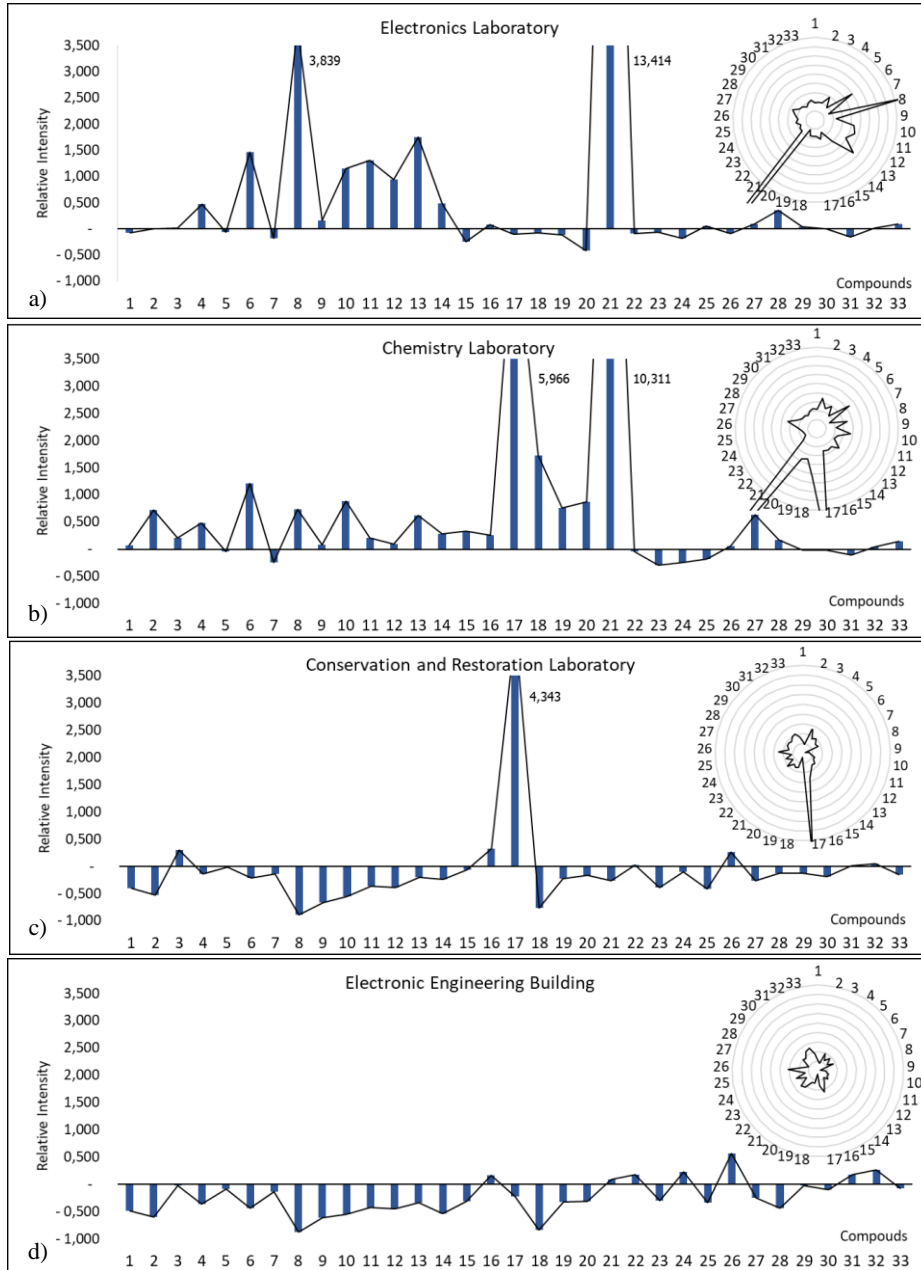


Fig. 2. Intensity profiles to some of the analysed locations across the campus (i.e. a) – Electronics Laboratory, b) – Chemistry Laboratory, c) – Conservation and Restoration Laboratory, d) – Electronics Engineering Building).

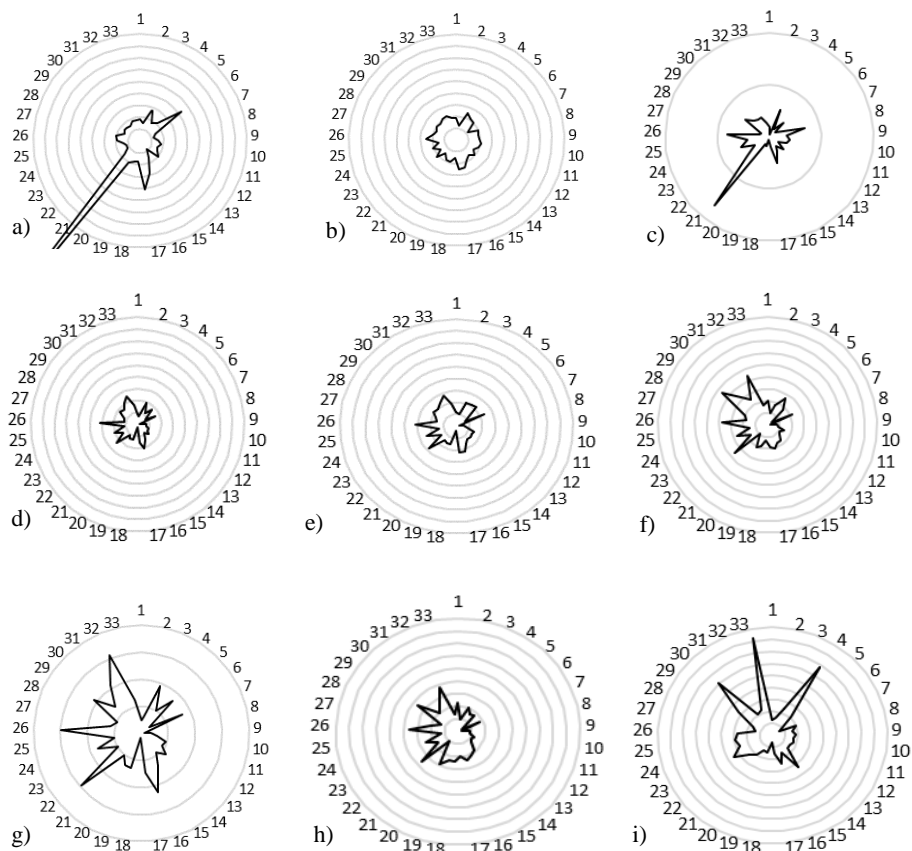


Fig. 3. Radar charts for the rest of the locations (i.e. a) – Administration Building Entrance, b) – Atomic and Molecular Physics Laboratory, c) – Biomechanics and Hemodynamic Laboratory, d) – Mechanical Engineering Building, e) – Fabrication Laboratory, f) – Canteen, g) – Parking Lot, h) – Material Engineering Laboratory, i) - Workshop).

5. Conclusions

From the visual analysis of bar and radar charts, a differentiation of intensity profiles for each location was allowed. This analysis indicates significant concentration differences of specific compounds between different locations of a same area which may reach dangerous levels. Such observations justify the crucial importance of environmental air studies as a scientific field.

Both the collecting and analysis methods were proven to be suitable to distinguish different intensity profiles of environmental air samples. With that in mind, it is possible to state that the GC-IMS technique is more than capable of identify and quantify possibly noxious VOCs to human health, in environmental air of distinct locations and qualitatively evaluate indoor and outdoor air.

To have a more detailed study, a wider range of locations with distinct characteristics should be included and analysed, and the identification of relevant compounds for this study should be conducted, as well as, their consequences to human health.

Acknowledgments. The authors would like to thank the Fundação para a Ciência e Tecnologia (FCT, Portugal) and **NMT, S.A.** for co-financing the PhD grant (PD/BDE/130204/2017) of the Doctoral NOVA I4H Program.

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Appendix

Table 1. Drift Time (sec.), Relative Retention Time, CAS Numbers and Notes for the identified compounds in all samples.

Peak Number	Drift Time (sec.)	Relative Retention Time	Identified Compound	CAS Number	Note
1	1,055	72,823	Ethanol	64-17-5	Monomer
2	1,127	93,108	1-propanol	71-23-8	Monomer
4	1,121	117,077	Ethyl Acetate	141-78-6	Monomer
7	1,284	246,377	Hexanal	66-25-1	Monomer
8	1,253	78,893	2-propanol	67-63-0	Trimer
9	1,103	79,330	2-propanol	67-63-0	Monomer
10	1,205	78,985	2-propanol	67-63-0	Dimer
14	1,158	87,569	Acetone	67-64-1	Dimer
16	1,077	120,420	2-Butanone	78-93-3	Monomer
18	1,149	71,803	Ethanol	64-17-5	Dimer
33	1,396	117,182	Ethyl Acetate	141-78-6	Dimer