



## Sequential discriminant classification of environments with different levels of exposure to tobacco smoke



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### HIGHLIGHTS

- A multivariate model is applied for the classification of environments.
- Three variables are required to classify types of smoking/non-smoking environments.
- Air exchange has a significant effect on the removal of highly volatile compounds.

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### ABSTRACT

The use of biomarkers permits the detection of smoking having taken place in an environment. However, no single biomarker is able to differentiate clearly between different types of environments. Multivariate classification models have helped us to differentiate between outdoors, non-smoking indoors, well ventilated smoking indoors, and smoking environments without good air exchange. We found that the variables that enabled us to classify environments most accurately were indoor temperature, 2,5-dimethylfuran and ethyltoluene. A successful prediction rate of 86.5% was obtained by applying both direct fitting and cross validation discriminant (leave-one-out) analyses. Our results show that although a good air exchange ratio decreases the levels of volatile organic compounds in indoor air due to tobacco smoke, significant contamination still remains.

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### 1. Introduction

The accurate determination of harmful substances in indoor environments is of great interest as people spend 70–80% of their time indoors in western populations (Lai et al., 2004; Simoni et al., 2003) and can be exposed to a range of indoor pollutants that may have adverse effects on health. Exposure to volatile organic compounds (VOCs) at large and medium levels can result in both acute and chronic health effects (Jones, 1999). Although there is no evidence of a health risk at the low levels normally detected in homes, some VOCs are well established carcinogens and genotoxins, for which safe levels cannot be defined, whereas others may be allergenics (IEH, 2001).

The focus of contamination studies changed at the end of the twentieth century when “receptor-oriented” approaches began to substitute conventional “source-oriented” ones (i.e., analysis of contaminants in obvious and generally highly contaminated sources) (Lioy, 2010; Ott et al., 2007). Receptor-oriented contamination studies require the appropriate measurement of pollutant concentrations at points where people are in direct contact with the contaminants. This approach also requires the evaluation of the portion of those particular substances that may affect human health. Although some important evidence of association with health problems has been found, most studies devoted to air contamination in non-industrial environments have the limitations of lacking detailed and systematic exposure measurement and, in many cases, of being observational studies (Brown et al., 2010; Bruce et al., 2002).

One of the most important indoor contaminants is environmental tobacco smoke (ETS), which can be inhaled by passive smokers (IARC, 2004; US-EPA, 1992; WHO, 2000). This is a complex mixture of gases and particles that has been classified as a Group A carcinogen (US-EPA, 1992). The gaseous phase of ETS includes hundreds of VOCs,

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some of which are also classified as carcinogenic individually (IARC, 2004). As a result, smoking has been heavily restricted in public places in most developed countries. ETS, or secondhand smoke, contains substances from two different sources: (i) mainstream smoke, which is generated during puff-drawing from the burning tip of the tobacco, and (ii) side-stream smoke, which is a combination of the smoke emitted into air during the burning of a tobacco product between puffs, the smoke escaping into the surrounding air during puffs, and the compounds of smoke that diffuse through cigarette paper (NCI, 1999). In those indoor areas where ETS has not been banned, it is often found to be the main indoor contaminant source of VOCs and it is therefore not necessary to be a smoker to be exposed to the harmful effects of tobacco smoke.

Many studies have been devoted to evaluating the levels of ETS exposure and finding appropriate ETS markers (Alonso et al., 2010a,b; Bi et al., 2005; Charles et al., 2007; Eatough et al., 1989; Hyvärinen et al., 2000; Kuusimäki et al., 2006; Rothberg et al., 1998; Vainiotalo et al., 2008; Xie et al., 2003; Zhong et al., 2007). The most widely evaluated marker of ETS exposure is nicotine, but the appropriateness of this has been questioned for different reasons. Nicotine is a semi-volatile compound and can be present in the air in both gas and particulate phases. Gas-phase nicotine exhibits different indoor behavior patterns from other ETS constituents (Löfroth, 1993, 1995; Nelson et al., 1992). Nicotine has been reported as being mainly in the vapor phase in side-stream smoke and mostly in the particulate phase in mainstream smoke (Eatough et al., 1989). It has the problem that it is easily adsorbed by a wide range of different materials (Daisey et al., 1994; Van Loy et al., 1997), resulting in a tendency to later reemission. Therefore, exposure emission factors increase over time (Singer et al., 2004). Given this, other more volatile compounds may be more appropriate for assessing direct exposure to ETS by passive smokers.

Nazaroff and Singer (2004) modeled the exposure intake of air pollutants from ETS for nonsmokers living with a smoker. They determined that, except for benzene, intake from residential ETS substantially exceeded intake from ambient sources and they estimated that exposure ranges from 0.1 to 14  $\mu\text{g}\cdot\text{m}^{-3}$  are to be expected in breathing zones. These values were determined assuming the presence of only one smoker and so higher levels can be expected in public indoor spaces where more than one smoker is present. In a study where the content of different VOCs related to ETS was evaluated in smoking and non-smoking premises (Alonso et al., 2010b), it was found that >48% of the smoking premises gave concentrations above the maximum estimated range by Nazaroff and Singer (2004), and more than 50% of the non-smoking premises gave values below their minimum estimate.

Ventilation rate is another important factor in determining the magnitude of indirect exposures. When ventilation rates are high, mass droops rapidly in indoor environments and most of the potential hazard is limited to direct exposure during the smoking period. Singer et al. (2003) determined that at a 2.1  $\text{h}^{-1}$  ventilation rate, more than 90% of daily exposure to VOCs occurred during the 4-h smoking period. However, the air change/extraction devices present in public premises tend to have a limited air-exchange capacity as they are mainly aimed at maintaining a comfortable temperature.

The single use of an ETS marker allows us to differentiate between smoking and non-smoking environments but does not help to identify those premises that have particularly serious health effects due to the presence of higher and more toxic levels of ETS. The aim of this study was to evaluate the possibility of classifying environments by analyzing different target VOCs and applying multivariable statistics.

## 2. Experimental

### 2.1. Chemicals

All reagents were reagent grade with  $\geq 99.0\%$  purity (Sigma-Aldrich, Steinheim, Germany). Stocks were prepared in cleaned 10 L Tedlar gas-

sampling bags (SKC, Eighty Four, PA, USA) filled with nitrogen (99.9990% purity, purified for hydrocarbons, oxygen and water vapor) by injecting 1–2  $\mu\text{L}$  of individual components. Calibration standards were prepared by taking a fixed volume of the stock gas with a gas-tight syringe and diluting to 10 L with purified nitrogen in a clean Tedlar bag. Stocks and standards were freshly prepared for each calibration. The stability of the target compounds in the Tedlar bags was evaluated and confirmed for the period used for storage.

### 2.2. Study site

The field study was carried out in 67 different environments (56 indoors and 11 outdoors) located in the province of Girona (north-eastern Spain). Samples were obtained between September 2009 and March 2010. Smoking was permitted at 41 indoor sites and prohibited at the other 15.

### 2.3. Sampling

Indoor sampling was performed at the center of each establishment at a height equivalent to the distance where a seated person would normally breathe ( $\sim 1.5$  m). Outdoor samples were taken at roads outside some of these premises. Temperature and relative humidity (RH) were also measured.

Samples of approximately 1 L of air were taken with a one liter gas-tight syringe (SGE JUMBO syringe, SGE Europe, UK) in approximately 30 s. The samples were then introduced and stored until analysis in a cleaned Tedlar bag. No losses from the syringes were detected. 750 mL of the sample was analyzed with a microtrap coupled to a GC–MS system no more than 2 h after sampling (Alonso et al., 2010b).

Each sampling bag was cleaned with purified nitrogen several times before samples were collected. The last portion of nitrogen used in the cleaning process was analyzed and no detectable background levels of the target compounds were found. Each bag was used for a maximum of five samples. The measurements were carried out between Monday and Friday during working hours.

### 2.4. Analysis of VOCs

For the analysis of air samples, an in-house capillary thermal desorption device connected to a GC (Focus GC, Thermo Scientific, Waltham, MA, USA) with MS detection (DSQ II, Thermo Scientific) was used (Alonso et al., 2009). Component separation was achieved by the use of a ZB-5ms column (30 m length, 0.25 mm ID and 0.25  $\mu\text{m}$  film-thickness) (Phenomenex, Torrance, CA, USA). The oven temperature program was: 40  $^{\circ}\text{C}$  held for 2 min, then ramped at 10  $^{\circ}\text{C}\cdot\text{min}^{-1}$  to 270  $^{\circ}\text{C}$  and held for 2 min. The MS analyses were carried out in a full-scan mode (scan range 40–200 amu). Electron impact ionization was applied at 70 eV. Purified helium carrier gas was used with a constant inlet pressure of 31 kPa. Chromatographic data was acquired using Xcalibur software (v. 1.4, Thermo Electron). Method detection limits (MDLs, for a sample volume of 750 mL) were 0.02  $\mu\text{g}\cdot\text{m}^{-3}$  for benzene, 2,5-dimethylfuran and toluene, and 0.05  $\mu\text{g}\cdot\text{m}^{-3}$  for ethylbenzene, *m*-, *p*-xylene, *o*-xylene, styrene, benzaldehyde, and 2-ethyltoluene.

### 2.5. Data analysis

Samples were classified in four groups according to the environments and environmental conditions evaluated: (1) smoking premises during mild/warm period ( $n = 21$ ), (2) smoking premises during cold period ( $n = 20$ ), (3) non-smoking premises ( $n = 15$ ), and (4) outdoor environments ( $n = 11$ ). A visual inspection of biplots revealed how simple combinations of pairs of variables accounted for feasible group partition, supporting the idea of generating discriminant models involving only a few variables. Three variables which intervened in a classification model obtained by the successive application of linear

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