Definition of simple, robust and industrialisable molecular criteria to predic olfactory perception and its hedonic component among different cultures

Vehicle Interior Air Quality (VIAQ) gets a growing interest among car manufacturers. On one side, legislations on Volatile Organic Compounds (VOC) becomes stricter. On the other side, vehicle odour represents an increasing concern for clients. These odours can be explained by the various composite materials inside a car. Usual chromatographic methods relying on Gas Chromatography (GC) already allow to detect the most abundant molecules. This is enough to quantify main pollutants or, occasionally, determine the molecule responsible of an abnormal odour in a car or material. However, materials with similar chromatograms may have very different odour. Most abundant molecules rarely explain global odour. Furthermore, the odour of a mixture of odorants cannot be simply explained by a sum of odours, it is necessary to understand the interactions between minor odorants. With current methods, it is impossible to anticipate the odour of a material from its emissions. Thus, understanding and anticipating odours requires new analytical techniques to undercover the true complexity of material emissions. To establish links between individually detected molecules and global material odour, we will also use human nose panels.

Firstly, we developed a new analytical technique relying on comprehensive bidimensional gas chromatography (GCxGC), allowing to detect up to several thousand molecules, combined with a thermodesorber for the injection (TD) and a time of fly mass spectrometer for the detection (ToFMS). Our complete TD-GCxGC/ToFMS system allowed us to identify several hundred molecules emitted by 8 representative car materials. Using the literature, we established a list of 191 odorous molecules from the emissions of 4 materials among the previous ones.

We presented these 8 materials and 10 odorous molecular referents – molecules with known odour – to a panel of untrained human noses, asking them to rate the pleasantness and intensity of the odours, while also describing those using olfactory poles. Simultaneously, we measured their respiration. Subjective pleasantness ratings allowed us to define two groups of materials, Neutral and Unpleasant. We then compared the objective olfactomotor data (inhalation time and volume...) and found a discrimination between the two groups. This effect had already been observed on reference pleasant and unpleasant odorants, but not on car materials, especially not without pleasant odorants.

We reproduced these sensory experiments with only 4 materials and no referent while recording cerebral activity by electroencephalography (EEG). Not all the results of the first experiment where observed again, which raises some questions about the presence of the other referent and the contrast they represent.

Finally, we established relations between the molecules detected in the 4 materials emissions and the descriptions made of the materials odour. Chemical emissions being very complex, we first used Principal Components Analysis (ACP) to determine the most discriminatory parameters. Then, we studied the relationship between the usage of certain groups of descriptors and the presence of certain groups of molecules. No individual molecule could explain the aspect of an odour, but their sum was able to. This original methodology can later prove to be very useful in the understanding of complex mixture odour.