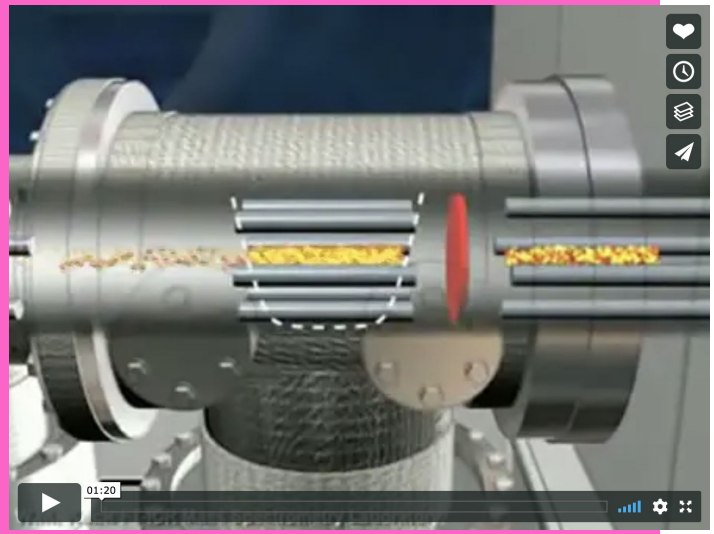
Mass spectrometry Animation from eLearn.Punjab on Vimeo.



Chemical Analysis
with speciation

Chemical analysis (with speciation) is a way of separating, identifying and measuring the different compounds that are present in a sample of odourous air. It is difficult to use this method to measure annoyance of odours as the presence of different chemical compounds can have different effects when combined with others - some combinations may intensify the odour whereas others may counterbalance.

What is it?

The chemical analysis (with speciation) of odorous emissions consists in the complete identification and quantification of odorous chemical compounds in an odour sample. It is an “instrumental analysis” because it investigates odour using instruments. Sensitive and powerful tools are required for odour analysis.

Different instrumentation can be applied for this purpose: the main technique Gas Chromatography coupled with Mass Spectrometry (GC-MS). GC - MS is a technique that combines the separation capability of gas chromatography (GC) with mass spectrometry (MS), which allows for the identification of the separated compounds *(Figure 2)*.

Gas chromatography can separate molecules depending on their chemical-physical properties: such as a foot race, molecules run along the GC column and they reach the MS detector in different time (called retention time), according to their chemical characteristics. This separation allows the MS to analyse molecules separately: indeed, mass spectrometer breaks each molecule into ionized fragments, obtaining a mass spectrum. A mass spectrum is a molecule fingerprint, that is characteristic and allows to identify uniquely a substance.

So, we obtain a chromatogram, a diagram where we can observe different peaks, each peak attributable to the different molecules separated by the GC column in function of time *(Figure 3)*. Under every chromatographic peak, it is possible to analyse the mass spectrum and identify every substance.

Background

Chemical analysis with GC-MS is an "old" and consolidated technique and is historically the first method applied for odour analysis. However, it cannot be considered as a method developed specifically for odour measurement. Although the type of information obtained with this kind of analysis can be very accurate, it's not directly related to odour perception.

What can it be used for?

At the emission level, GC-MS can be applied in order to obtain information about the chemical composition of odour emissions. GC-MS allows for the identification and quantification of complex odour emissions. Identification and quantification of the chemical compounds that are present in an odour emission are fundamental to evaluate the impact of emitted compounds on the environment and human health.

Chemical characterization also allows to evaluate compliance of the emissions with regulatory concentration or flux limits that are fixed by the competent authorities in order to protect workers and citizens from exposure to hazardous or toxic compounds.

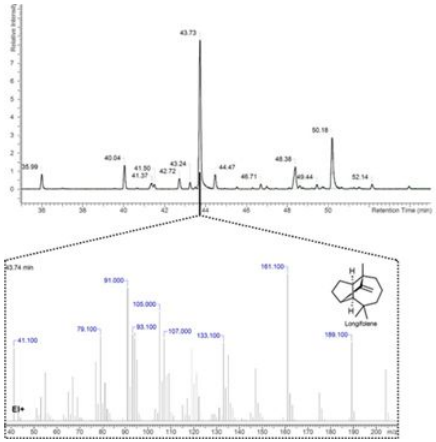


Figure 2.

What can it NOT be used for?

Chemical analysis can turn out to be very difficult and not always effective, especially in the characterization of complex odours. Odours are not additive: in odorous mixtures, synergistic and masking effects between different odorants may occur, giving that the chemical composition of an odorous sample can not be related to its odour concentration.

One way to relate the chemical composition of an odorous mixture to its odour concentration is to evaluate the so called "Odour Activity Value" (OAV), which is calculated as the sum of the ratio between the chemical concentration of each compound in the mixture and its odour threshold concentration:

- OAV = Odour Activity Value (ouE m-3)
- Ci = Concentration of compound i (mg m-3)
- OTi = Odour Threshold of compound i (mg ouE-1)

However, the odour concentration calculated through the OAV can be very imprecise. One reason for this imprecision is the difficulty of finding reliable OT values, given that the values that are found in literature for a single odorous compound often differ by several orders of magnitude. Moreover, if synergic effects of odorous compounds are present, such a calculation will underestimate the odour concentration of the odorous mixture.

Finally, analytical techniques are not as sensitive as human nose to detect all malodorous compounds. Indeed, there are some odorous compounds that have odour threshold concentrations in the range of ppb (parts per billion) o even ppt (parts per trillion), which are levels that are hardly detected by instrumental methods.