QIC - 20
Fragrance Fingerprinting

Summary

The Hiden Gas Analysis system, QIC-20 was used to analyse and identify the headspace of various fragrances.

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Introduction

Fragrances are commonly used in many household products to improve the pleasure of use. There are often several active components together with volatile chemicals and other organic molecules that comprise the fragrance.

A typical method for analysis and quality control is gas chromatography, GC, sometimes coupled with mass spectrometry, GC-MS. Sample preparation for both these methods is slow and the analysis procedure may take several hours also. This limits the usefulness of these techniques.

Hiden Quadrupole Mass Spectrometers (QMS) allow a quicker and easier way to analyse such complex fragrance mixtures. A complete gas analysis system or dissolved species system can rapidly examine many samples.

In this particular application the requirement was for quality control, so that the data required was needed to compare the sample with a quality standard, using a difference spectrum.

Experiment

Various fragranced samples were analysed. The first method was directly sampling the fragrance headspace, using the end of QIC inlet positioned close to the sample. For less viscous samples, a small amount was poured into a test tube. Using a bubbler, the headspace was kept at atmospheric pressure.

Lavender oil is a concentrated fragrance comprised of two main components, Linalol and Linalol Acetate. To scan for just for the major/molecular ions of the species, scans were taken using the gas analyser soft ionisation mode, ref app note 250, soft ionisation for simplified mass spectra.

In Figure 1, three cycles, nos. 1, 5 and 10 are seen. As each cycle took approximately 1 minute, just 5 or 10 minutes collects sufficient data to identify the main components.

After just 5 cycles the key peaks at 136 and are becoming visible. After 10 cycles, other minor components are visible, at 191 and 193 amu.

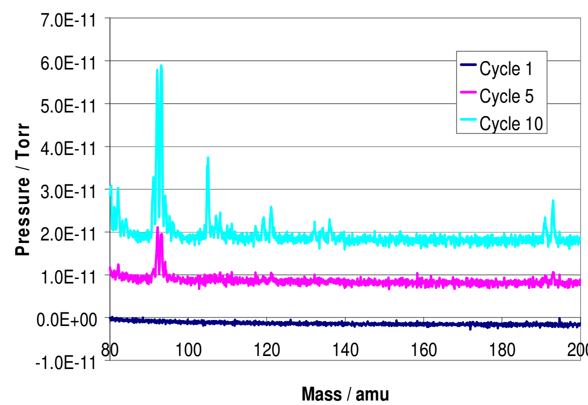

Figure 1: Profile accumulate scan of Lavender oil. (Offset introduced to clarify cycles).

The speed of response, and specificity are the main advantages of the direct inlet mass spectrometer technique. Another advantage is that continuous on-line sampling over long periods is a standard operating mode of the Hiden system. This is useful for the monitoring of the decay of fragrance strength with time, as evaporation occurs. In this case, multiple ion detection, MID mode was used, selecting various ions corresponding to the masses of the fragrance molecules. This was investigated using a cloth soaked with a 0.5% solution of a fragrance. The results are seen in Figure 2.

The main peaks present corresponded with Geraniol, a common fragrance component. The cloth was analysed over time. As can be seen, the fragrance strength first increases, indicating that more of the fragrance evaporates and is detected. After more time this will decrease to background levels.

A third experiment that was performed was a comparison of similar products with different fragrances. The mass spectrum of this product is quite complex, as contributions from the bulk compound and also the fragrance components are present. However, when this is subtracted from another product, the bulk compound signal is removed, and the difference between the two spectra is left. This is the fragrance.

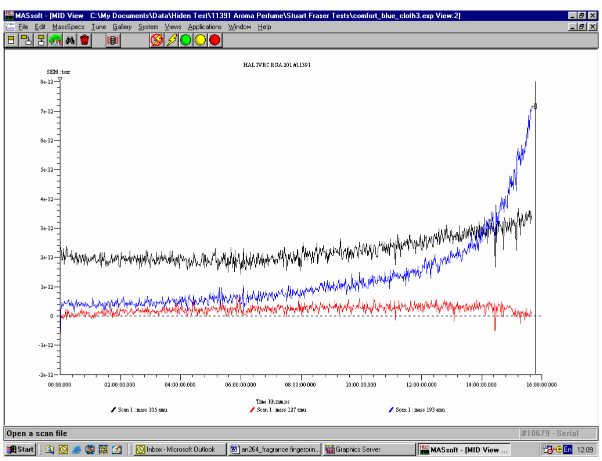

Figure 2: MID scan of Geraniol based fragrance.

Figure 3 shows an example of a difference spectrum. The peaks above the zero line are from one fragrance, and the peaks below the zero line are from the other fragrance. The main peaks can be identified as benzyl alcohol (a volatile chemical which acts as a carrier for the fragrance) and Geraniol (a common constituent of fragrances).

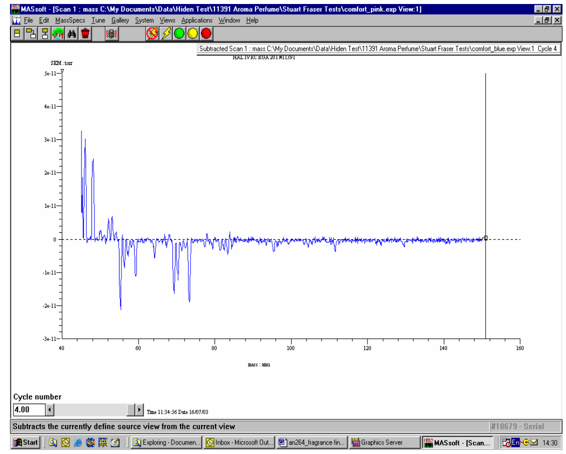

Figure 3: Subtracted Profile scans for two similar products with different fragrances.

Hence the HPR-20 system covers a variety of applications within the fragrance industry and could prove a valuable piece of analysis equipment.

Conclusion

Direct inlet Mass Spectrometer can effectively detect low levels of the fragrance organic molecules. Using a comparative method the direct inlet mass spectrometer can effectively identify the presence and quantity of fragrance components. Therefore Mass Spectrometry adds new potential to the current analysis techniques of gas chromatography and fragrance recognition (‘electronic nose’) technology.