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DETECTION OF THE MOLD MARKERS USING ION MOBILITY SPECTROMETRY

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ABSTRACT

Microbial contamination can be harmful for the human health. Usually the fungal growth is indicated by a higher concentration of microbial volatile organic compounds which is produced by molds in the indoor air. Such molds can cause a large variety of health problems such as skin and eye irritations, allergic reactions, headaches, breathing difficulties, and amplification of asthma symptoms [1]. Examples of the most frequently reported microbial volatile organic compounds in the literature include 1-octen-3-ol, 2-methyl-1-propanol and dimethylsulfide and these have been detected in air using ion mobility spectrometers equipped with different ionization sources (UV-discharge lamp and ^{63}Ni-radioactive foil). The detection limits were found in the range of ng/L using ß-radiation (^{63}Ni) and in low µg/L-range using a 10.6 eV UV - lamp as ionization sources. For the analysis of mixtures, UV-IMS was combined with a conventional gas chromatographic column. The results of the successful detection of emissions of bread mould cultures measured with different IMS analyzers will be shown with respect to the practical applicability of the procedure with real samples. Advantages and disadvantages of the method presented will be discussed in detail. To approve IMS-findings, results were compared with measurements using GC-mass spectrometry.

INTRODUCTION

Airborne fungal contaminants in buildings are widely discussed vis-à-vis health hazards for occupants. In the climate of Europe, ~10 to 20 per cent of all dwellings are affected by excessive formation of mold. Microbial volatile organic compounds (mVOCs) arise from the metabolic activity of the fungi and include alcohols, terpenes, ketones, aldehydes, esters, aromatic and sulphur containing compounds. Some of these compounds, such as 1-octen-3-ol produce a specific earthy odor, which is detectable before any visible sign of the mold. When airborne concentrations of these or other mVOCs rise to hundreds of µg/m^3, humans can be irritated by unpleasant odors [2].

In order to determine mVOCs in ambient air, variations in concentrations may arise from building use, variations of vapor sources, process conditions, and other environmental factors and suitable analytical monitoring of these may required a continuous and fast chemical analyzer. Ion mobility spectrometry will permit routine determinations of mVOCs in air and provide fast results in range of milliseconds to several minutes. Since the detection limits of the mVOC reach to the ppt$_v$ range by IMS, on-site measurements of these compounds should be plausible. On-site and facile monitoring of such substances would also aid the identification of areas of fungal blooms and the abatement of these health risks. The purpose of these studies is to assess various configurations of mobility spectrometers and sampling strategies relevant to monitoring mVOCs in ambient air of indoor atmospheres.

METHODS AND MATERIALS

GC-UV-IMS

An IMS drift tube made in-house with a 10.6 eV UV lamp as the ion source [3] was coupled to a Hewlett-Packard model 5890A gas chromatograph (GC). A heated stainless steel line was used to join capillary column to the IMS ion source so that substances eluting from the GC would be passed from GC to IMS without complication of condensation in an interface. The operating conditions of the GC were: Column- MXT®Volatiles (Silcosteel), 30 m / 0,53 mm / 2 µm (Restek GmbH, Bad

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Figure 1: Sampling using a SPME fiber (left) and direct measurement using ^{63}Ni-IMS

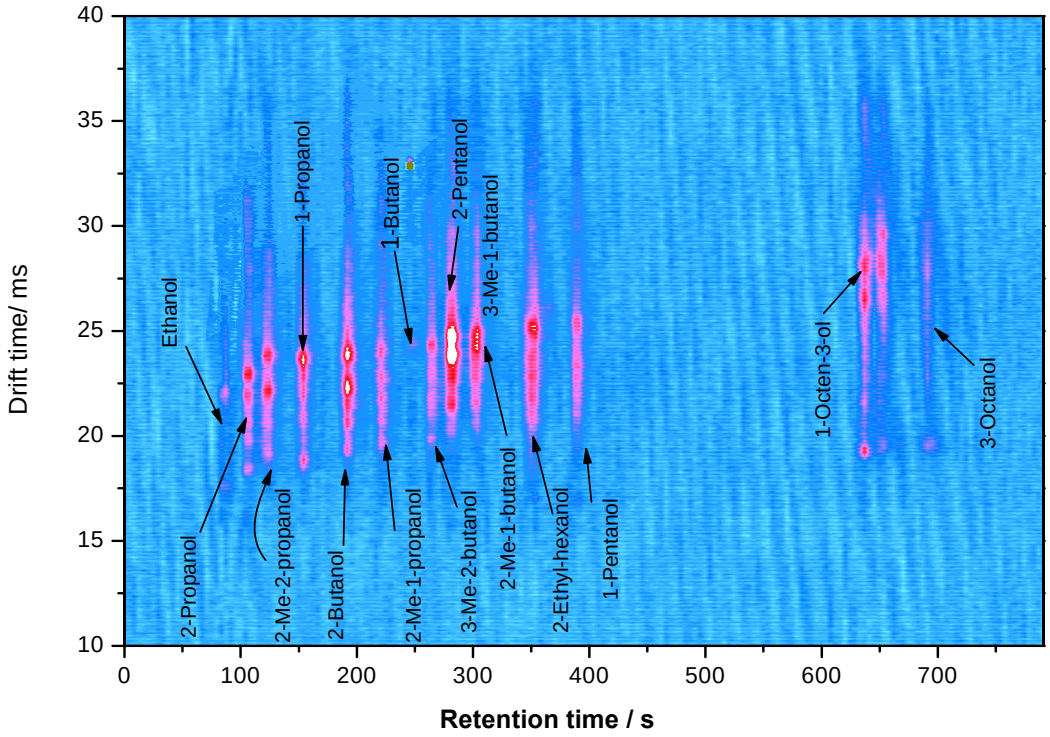

Figure 2: Separation of 15 alcohols using a home made 10.6 eV GC-UV-IMS

Homburg, Deutschland), temperature program- Initial temperature: 30 °C, initial time: 1 min, column oven program rate: 10 °C/min to 150°C and then 15°C/min to 200°C, and final time, 2 min. The injector temperature was 200 °C and the transfer line was heated to 150°C.

Testgases

For 22 different mVOCs selected, which are the most frequently produced by mold in the indoor air, ion mobility spectra were obtained using IMS drift tubes with UV and with radioactive ionization sources. Test gases were prepared using neat liquid substances in permeation tubes. Synthetic air was used as sample and drift gas for the ^{63}Ni-IMS and nitrogen was used for measurements with the UV-IMS.

Bread mold cultures

About 100 g of a light-brown bread was placed in glass flask, capped, and stored 35 days. Moisture was measured as 95 percent the beginning of bread storage and was maintained during the whole experiment by

Table 1: Summary of mobility values and retention times of the MVOCs selected

Substance	Retention time [s]	Mobility (K_0) [$cm^2/(vs)$]				
		>1.9	1.9-1.7	1.7-1.5	1.5-1.2	>1.2
Ethanol	83		**1.82**, 1.71		1.47	
Acetone	103		1.73			
1-Propanol	144		1.72	**1.53**	1.40	
2-Propanol	100				**1.40**, 1.36	
1-Butanol	255			1.64	**1.41**, 1.36	
2-Butanol	187			1.69, **1.51**	1.37	
1-Pentanol	379	1.94		1.56	**1.30**	
2-Pentanol	287			1.61, 1.52	1.41, **1.36**	
2-Methyl-1-butanol	341			1.60	1.46, 1.37	
3-Methyl-1-butanol	336			1.55	**1.30**	
3-Methyl-2-butanol	269				1.36	
2-Me-1-propanol	212			1.65	**1.42**, 1.36	
2-Me-2- propanol	117				**1.45**, 1.36	
2-Methylfuran	183	**1.98**			1.40, 1.21	
3-Octanon	636				1.23, **1.25**	
1-Octen-3-ol	620			1.69	1.24	1.15, **1.11**
3-Octanol	636			1.66		1.18, **1.11**
2-Ethyl-hexanol	377			1.66		1.18, **1.10**
Cyclopentanon	262				**1.49**, 1.41	
a-Pinen	562			1.64		**1.18**
Anisol	575			**1.66**	1.20	1.17
Longifolen	1.080				1.39	0.93

adding of some water. Emissions of the culture were measured directly using ^{63}Ni-IMS and using solid phase micro-extraction (SPME) fibers (CAR-PDMS-fiber) for GC-UV-IMS. Times for sampling with SPME were 30 min. Samples and analyses were in the same day so comparisons between IMS analyzers could be made with uncertainties of sample storage.

RESULTS AND DISCUSSION

The reduced mobilities of positive ions from individual compounds were calculated using ion mobility spectra and results are shown in Table 1. The mVOCs most often detected during these studies were alcohols with small molar mass. These exhibited more than one peak in a spectrum and exhibited mobility values characteristic of fragment ions. The K_0 values belonging to the highest peak of the mobility spectra are marked with bold letters in Table 1. The ions with mobility values below 1.5 cm^2/Vs should contain some water molecules. The complexity of these mixtures and the extensive fragmentation of alcohol ions made the spectra difficult to interpret and the analytical results problematic. Consequently,

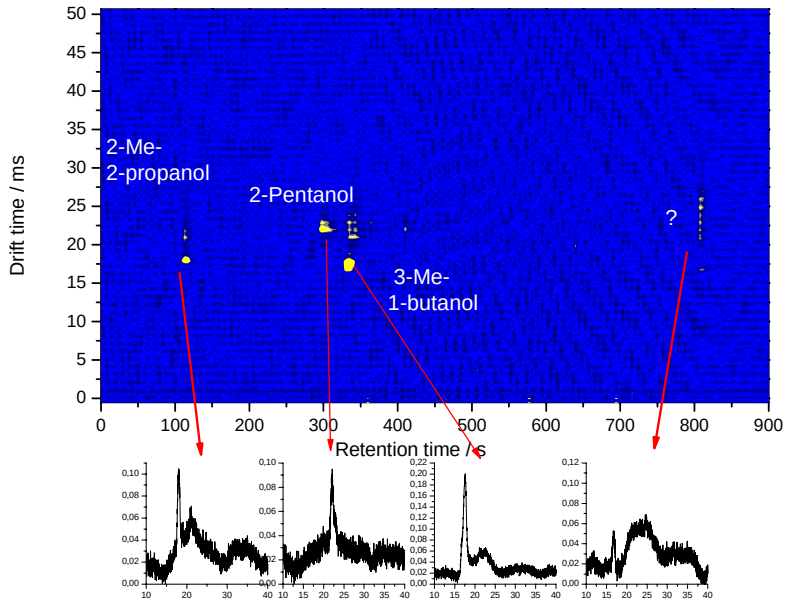

Figure 3: 2D-plot of bread mould culture measured by GC-UV-IMS

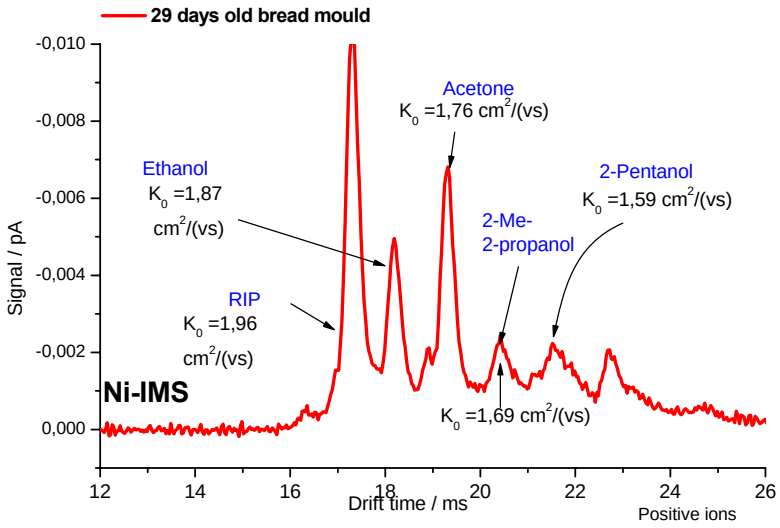

Figure 4: Ion mobility spectra of 29 days old bread mold culture used ^{63}Ni-IMS

direct sampling was replaced with a chromatographic separation of the sample.

Samples using the SPME fiber were drawn from headspace over individual neat substances with an adsorption or sampling time of 2 min. These were thermally desorbed and measured with a GC UV-IMS built inhouse with a 10.6 eV photo-discharge lamp for the ion source. Results for retention times of these chemicals were well-defined and are shown in Table 1.

A mixture from all alcohols was prepared, sampled and analyzed using identical method as that for the individual substances. Results from these GC-IMS experiment are shown in Figure 2 where the separation of 15 alcohols in 10 minutes is shown.

A first experiment with a culture of bread mold raised in the laboratory was made to identify some mVOCs from the sample with the help of different IMS analyzers. Samples were taken every third and seventh day weekly and were measured using the GC UVIMS and the ^{63}Ni-IMS.

A 2D-plot from the emission from a 29 day old bread mold culture is displayed in Figure 3. From the MVOCs detected in this sample, 2 - methyl-2 propanol, 2-pentanol and 3-methyl-1 propanol were identified based upon retention time and mobility spectrum. These identifications were confirmed using GC-mass spectrometry.

In Figure 4, an ion mobility spectrum is shown from the direct analysis with ^{63}Ni-IMS of the same mold culture as that shown in Figure 3. In addition to ethanol (K_0 = 1.87 cm^2/Vs) and acetone (K_0 = 1.76 cm^2/Vs), other peaks can be seen and these were recognized, mostly likely, as alcohols, including 2-methyl-2-propanol (K_0 = 1.69 cm^2/Vs), and 2-pentanol (K_0 = 1.59 cm^2/Vs).

Without a pre-separation step, an exact analysis of such a complex sample is difficult, and comparisons with other methods are needed. However, direct measurements using the ^{63}Ni-IMS offered simple, direct, and fast screening. This could find value in on-line monitoring of the air quality for presumptive analysis of indoor air quality on a continuous basis.

CONCLUSIONS

Ion mobility spectrometers equipped with radioactive and also UV photo-discharge ionization sources were successfully used for

the determination of mVOCs from actual mold samples. The drift tube with a ^{63}Ni ion source exhibited low detection limits for alcohols and suggested the possibilities for a continuous on-site monitor of indoor air quality. However, pre-fractionation using gas chromatography offers analytical value with such complex samples. In the future, the combination of IMS with a high speed multi-capillary column might result fast analysis with exact identification of microbial air pollutants. These findings demonstrate that emissions of mVOCs from various mold cultures could provide mass fluxes suitable for fingerprinting of various species[4] and might be useful for source assignments or discovery of fungal contamination in indoor environments of buildings.

References

[1] Dewey et al., 1995, Larsen and Frisvad, 1994, Böck et al.,1998, Wessen et al.,1995, Fischer et al.,1999

[2] Fiedler, K. Schütz, E. Geh, S.: Detedtion of microbial volatile organic compounds (MVOCs) produced by moulds on various compounds, Int. J. Hyg. Environ. Health 204, 111-121, 2001

[3] Baumbach, J. I. and G. A. Eiceman: "Ion Mobilty Spectrometry: Arriving On Site and Moving Beyond a low Profile." Applied Spectroscopy 53(9): 338A-355A.,1999

[4] Fischer G., Müller T., Schwalbe R.: Exposure to airborne fungi, MVOC and mycotoxins in biowaste-handling facilities, Int. J. Hyg. Environ. Health 203, 97-104, 2000