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THE QUEEN'S AWARDS FOR ENTERPRISE: INTERNATIONAL TRADE 2015

Thermal desorption applications

IngenieríaAnalítica
Chromatography & Spectrometry

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Application areas

Environmental monitoring

Biological profiling

Automotive studies

Defence & Forensics

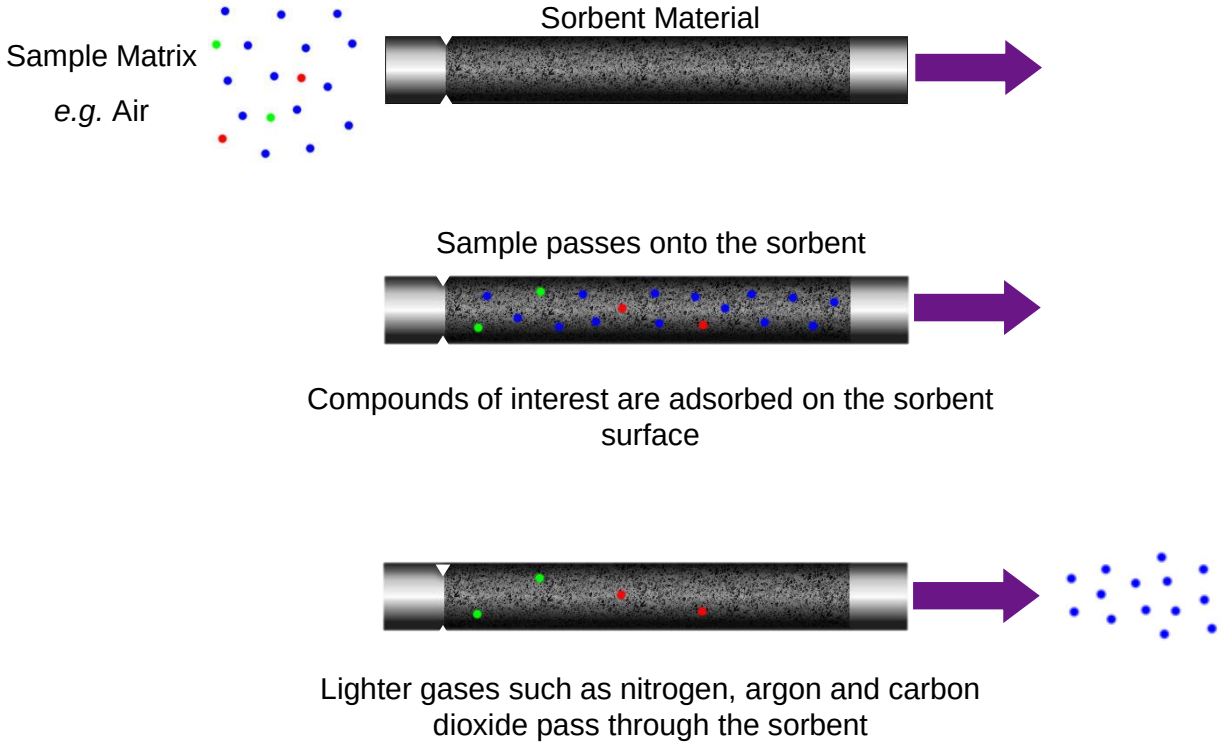
Fragrance & odour profiling

Consumer environmental health

Food & Drink

What is thermal desorption (TD)?

Sample collection



Challenges with air sampling

1. Many compounds are harmful at very low concentrations
   - ✓ Pre-concentration (Thermal Desorption)

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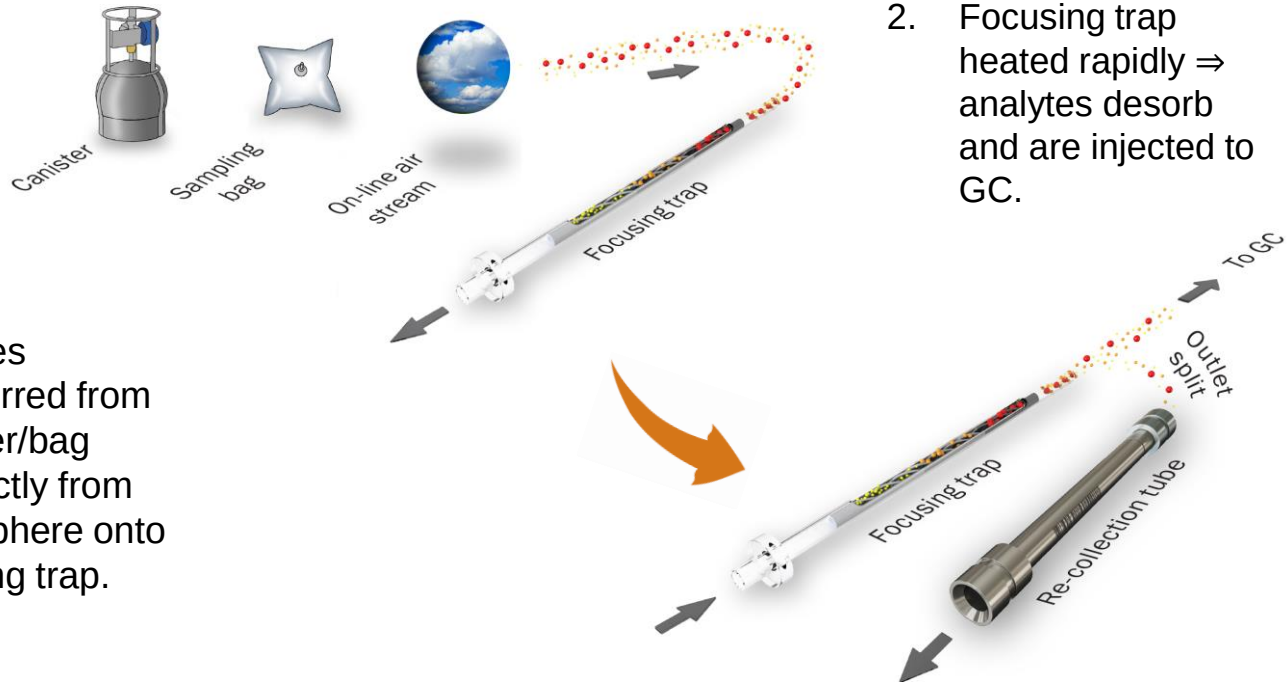
2. Many pollutants are very volatile – how can we collect and concentrate them?

‘Whole air’ sampling for very volatile samples

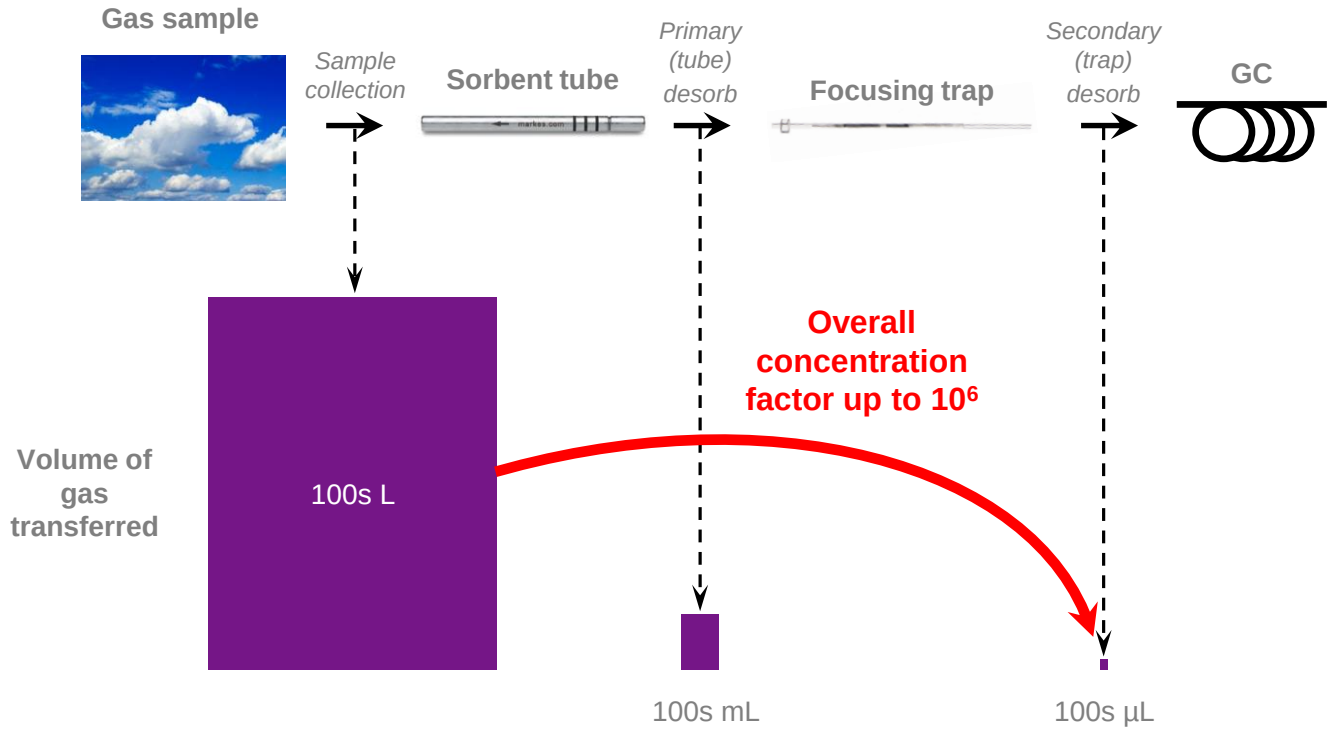
How it works



1. Volatiles transferred from canister/bag or directly from atmosphere onto focusing trap.

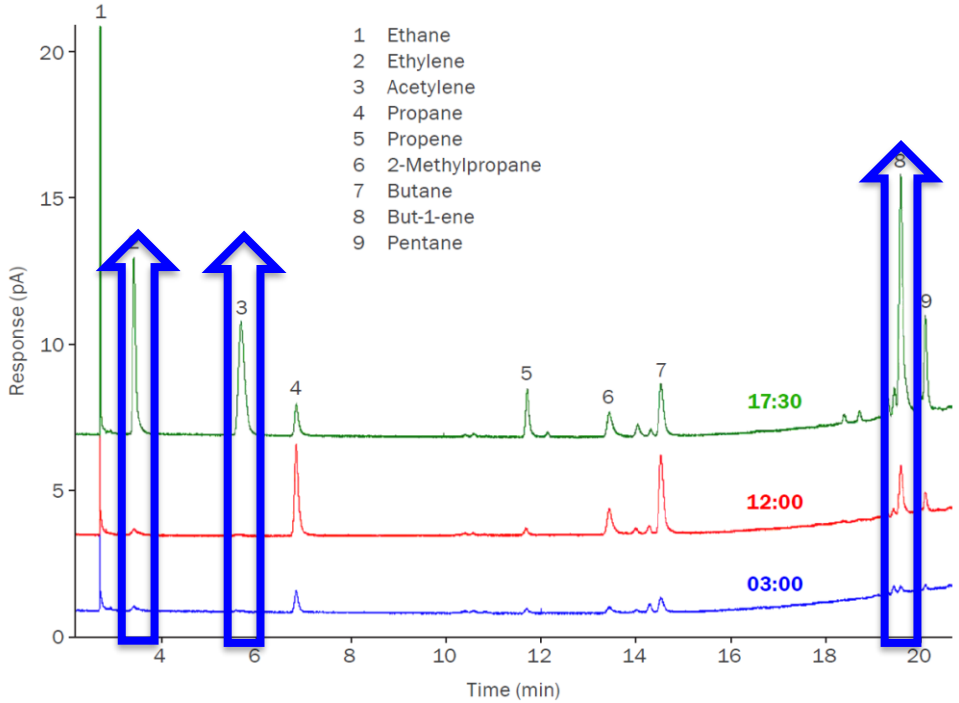
2. Focusing trap heated rapidly ⇒ analytes desorb and are injected to GC.

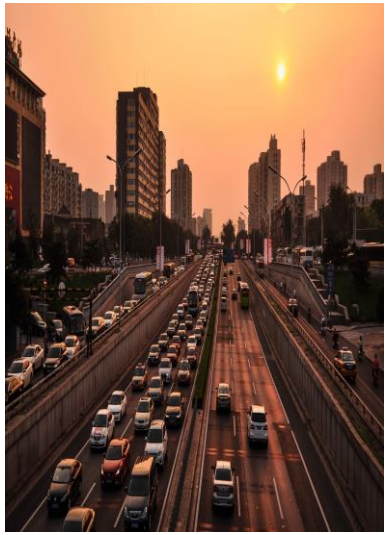
What is thermal desorption?



On-line pollution monitoring

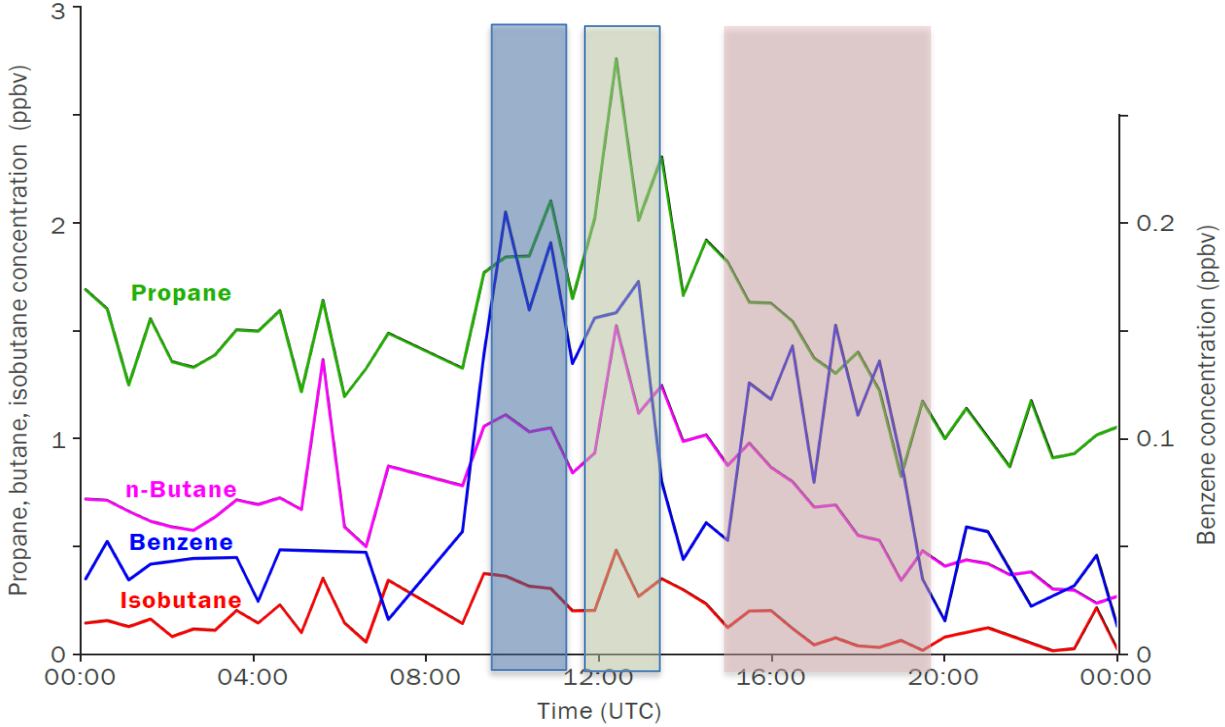
Very volatile ozone precursors





On-line pollution monitoring

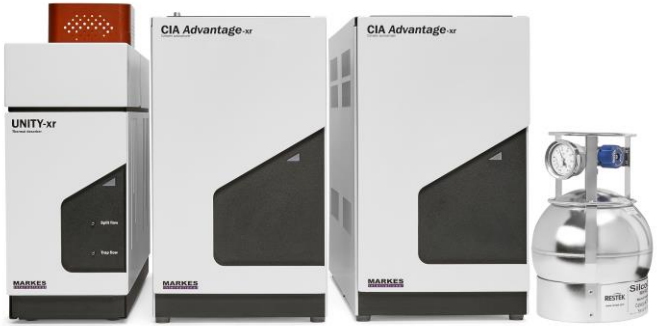
Diurnal variation in pollutant concentrations



Challenges with air sampling

1. Many compounds are harmful at very low concentrations
   - ✓ Pre-concentration

2. Many pollutants are very volatile – how can we collect and concentrate them?
   - ✓ Cryogen – free on-line or canister sampling
   - ✓ Selection of the optimum sorbent configurations



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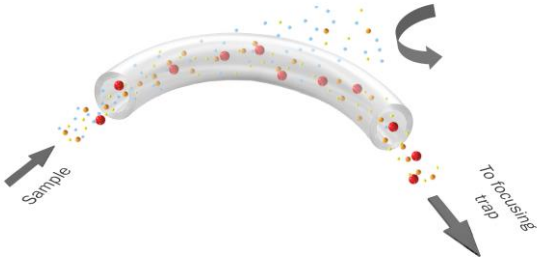
3. Air samples can be very humid – how do we remove water without removing compounds?

Water management techniques for air samples

Analyte type	Dry purge only
C2 compounds (VVOC)	×
C3+, Non-polar VOCs	✓
Pinenes	✓
Polar VOCs	✓
Sulphur compounds	✓

Water management techniques for air samples



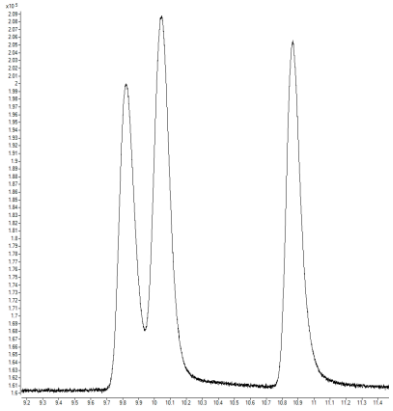
Analyte type	Dry purge only	Membrane dryer
C2 compounds (VVOC)	×	✓
C3+, Non-polar VOCs	✓	✓
Pinenes	✓	×
Polar VOCs	✓	×
Sulphur compounds	✓	✓

Water management techniques for air samples

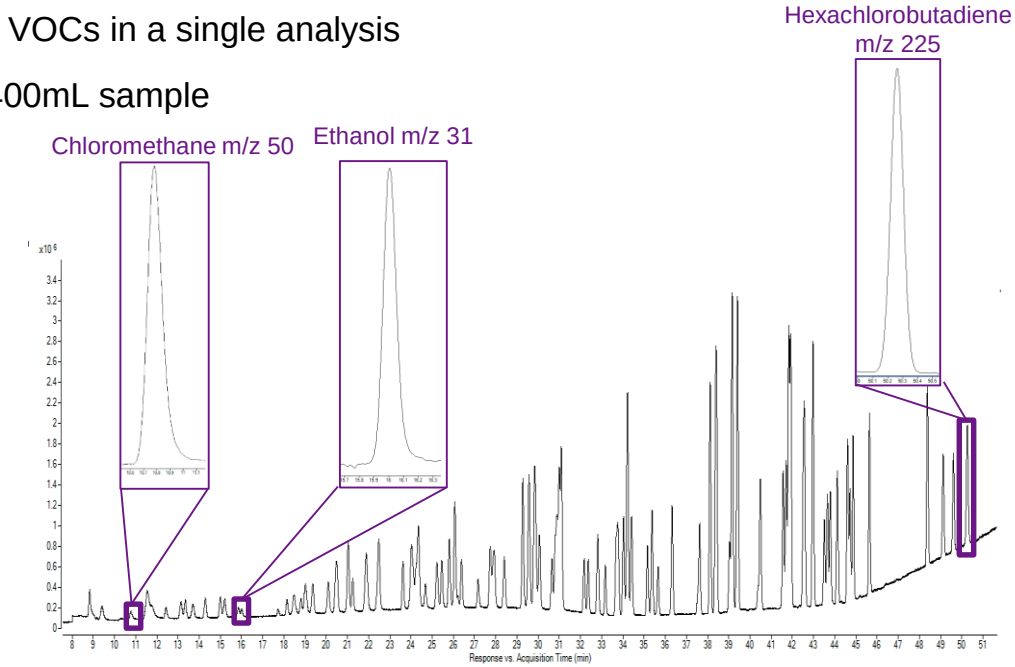
Analyte type	Dry purge only	Membrane dryer	Kori-xr
C2 compounds (VVOC)	×	✓	✓
C3+, Non-polar VOCs	✓	✓	✓
Pinenes	✓	×	✓
Polar VOCs	✓	×	✓
Sulphur compounds	✓	✓	✓

Cryogen-free combined ozone precursor & TO15 analysis

- Canister or on-line sampling of 108 pollutant compounds
- Cryogen free pre-concentration AND cryogen free chromatography
- 100% RH - VVOCs, OVOCs and VOCs in a single analysis
- Sub ppb detection limits from a 400mL sample



Ethene, Acetylene, Ethane to FID

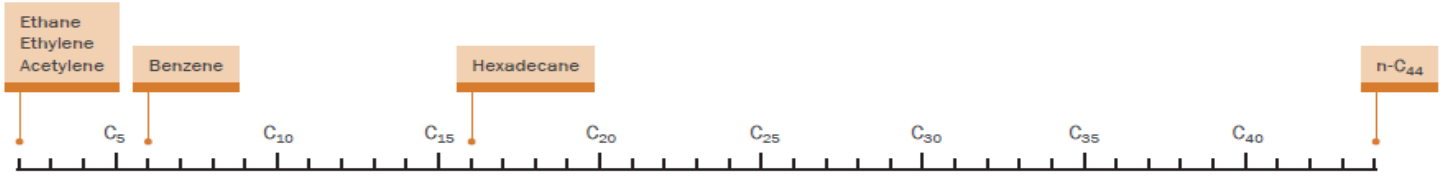


C_3 onwards to Mass Spec

Challenges with air sampling

1. Many compounds are harmful at very low concentrations
   - ✓ Pre-concentration
2. Many pollutants are very volatile – how can we collect and concentrate them?
   - ✓ Cryogen – free on-line or canister sampling
   - ✓ Selection of the optimum sorbent configurations
3. Air samples can be very humid – how do we remove water without removing compounds?
   - ✓ Water management technologies – sorbent selection, dry purge, membrane drying or kori-xr
4. I need to analyse SVOCs as well as VOCs
5. I need to sample at numerous remote locations

Techniques for air sampling and analysis

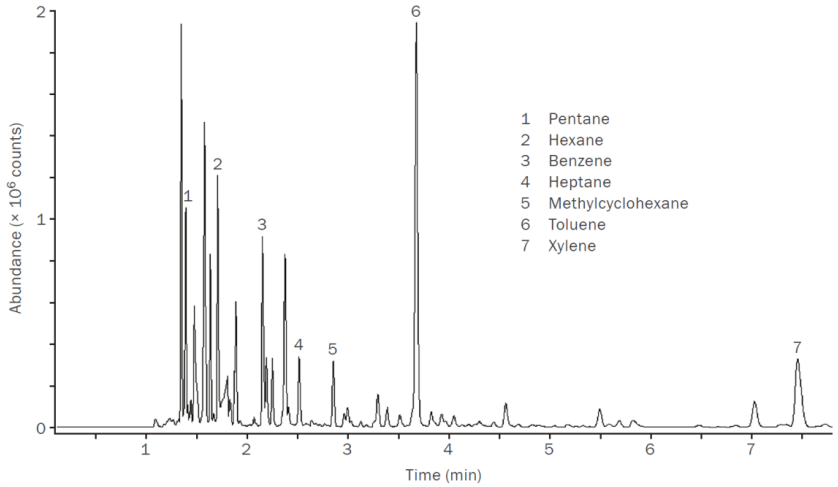


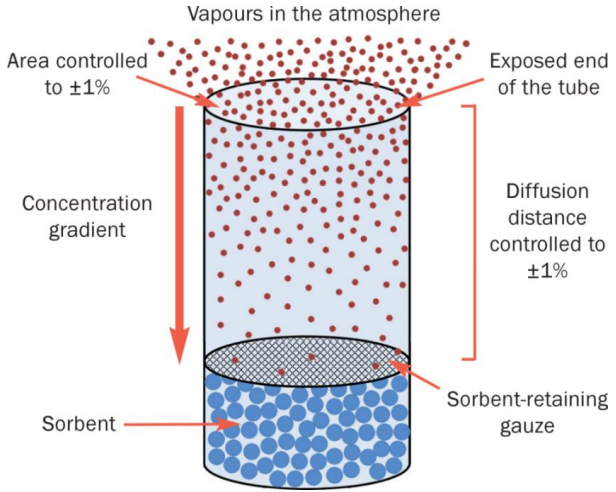
Canisters

On-line

Sorbent Tubes

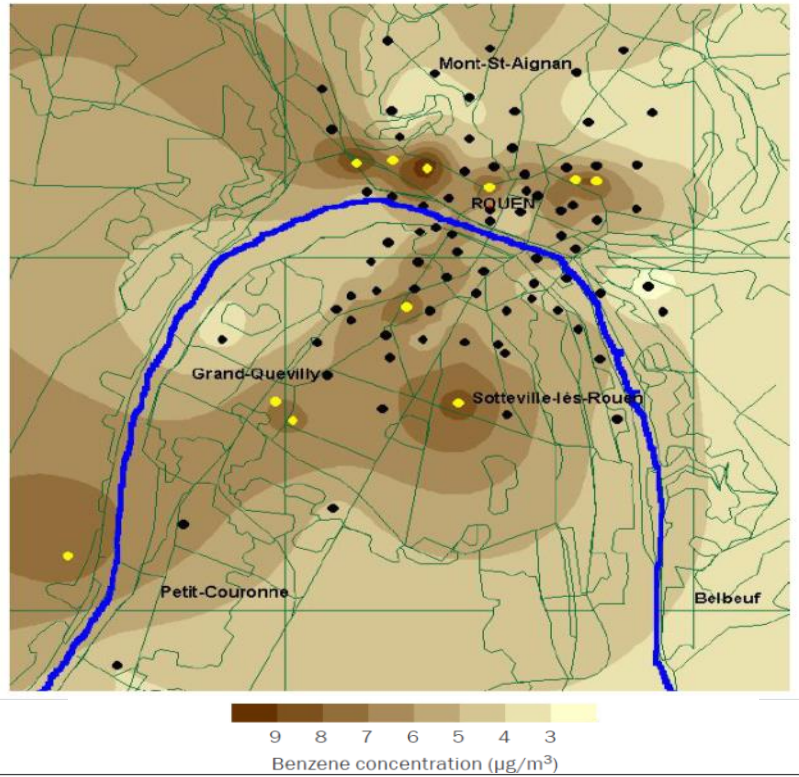
Sorbent tube sampling: Passive





Sorbent tube sampling: Passive

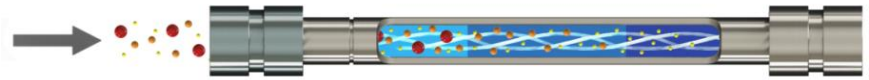
Five-day monitoring of benzene near Rouen, France



- 5 days
- Over 90 passive samplers
- Easy to deploy
- Unattended sampling
- 100 tube autosampler = unattended analysis

Sorbent tube sampling: Pumped

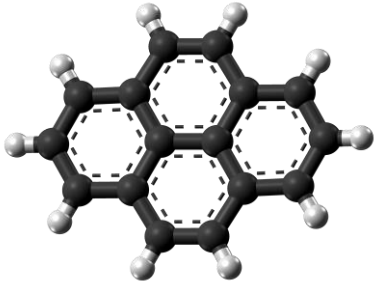
- A pump actively draws the air through the sorbent tube

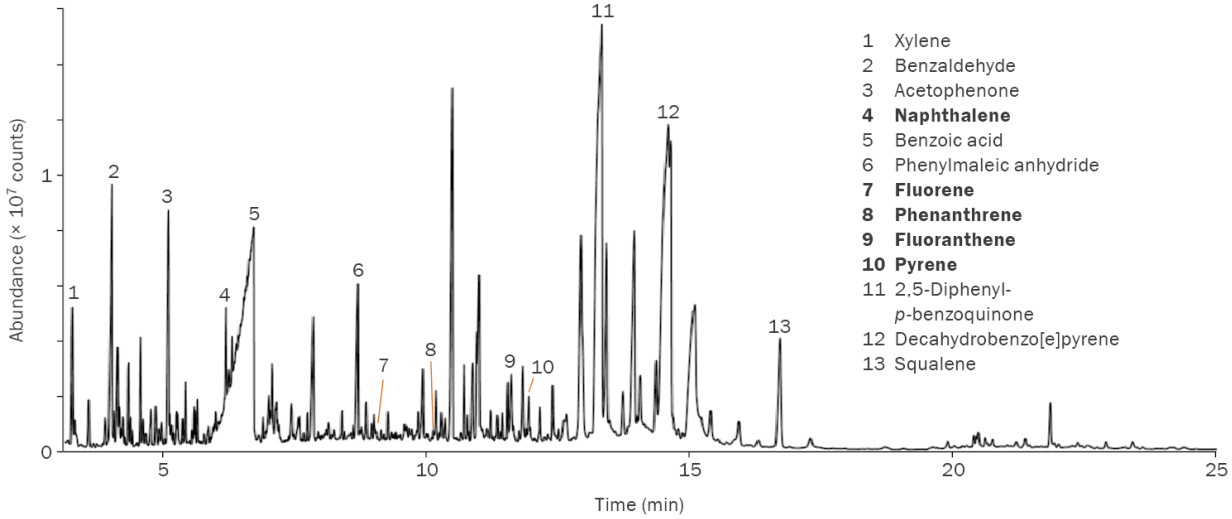


PUMP

Sorbent tube sampling: Pumped

- **180L** of Shanghai air collected on a sorbent tube
- 250 ml/min sampling for 12 h
- Many PAH compounds identified





Challenges with air sampling

1. Many compounds are harmful at very low concentrations
   - ✓ Pre-concentration

2. Many pollutants are very volatile – how can we collect and concentrate them?
   - ✓ Cryogen – free on-line or canister sampling (C_2 – C_{14})
   - ✓ Selection of the optimum sorbent configurations (C_2 – C_{44})

3. Air samples can be very humid – how do we remove water without removing compounds?
   - ✓ Water management technologies – dry purge, membrane drying or kori-xr

4. I need to analyse SVOCs as well as VOCs
   - ✓ Sorbent tube sampling ($C_{2/3}$ – C_{44})

5. I need to sample at many remote locations
   - ✓ Sorbent tube sampling ($C_{2/3}$ – C_{44})

The complete air monitoring solution

- ✓ Cryogen-free trapping of very volatile C2 hydrocarbons
- ✓ Automated analysis of 100 sorbent tubes AND up to 27 canisters or on-line samples in the same sequence
- ✓ Advanced water removal with dry purge and kori-xr

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Wider application of Thermal desorption

Consumer environmental health (CEH)

What is the focus?

- Potential health risks that arise from poor indoor air quality have prompted regulation of a wide range of materials
- The average American spends 93% of their time indoors…
- 86% in houses, offices, etc…
- … and 7% in automobiles.
- The majority of items which can effect the air quality in these locations are now regulated

Sampling and Analysis options

1 Indoor air monitoring

2 Final product certification

3 Screening of emissions from components

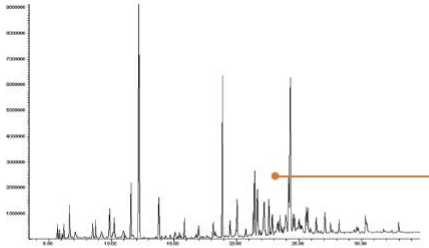
A Pumped sampling

B Small chambers

C Microchambers

D Direct desorption

The four main sampling approaches for assessing emissions from products and materials are all compatible with TD.



Analysis by gas chromatography

TD-based approaches can detect:

- **VOCs** (boiling up to n-C_{16}).
- **SVOCs** or FOG compounds (boiling above n-C_{16}).
- **Odorous** or **reactive** species.

Formaldehyde monitoring

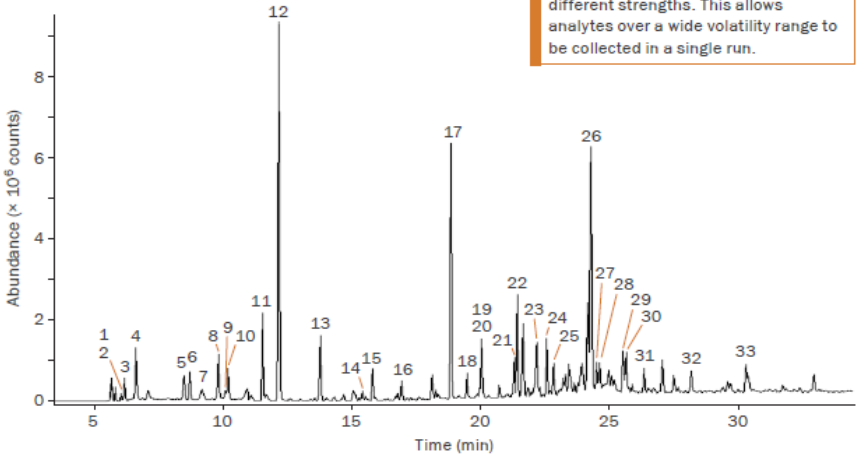
Note that formaldehyde and other aldehydes, unlike other VOCs/SVOCs, are analysed by HPLC rather than GC–MS, and require special sampling and analysis equipment such as DNPH cartridges. See page 20 for more information.

Indoor air quality

Assessing the cause of poor indoor air quality

1 1,1-Difluoroethane
2 1,1,1,2-Tetrafluoroethane
3 Dichlorodifluoroethane
4 1,1-Difluoro-1-chloroethane
5 Isopentane
6 Ethanol
7 Trichlorofluoromethane
8 Propanol
9 Freon® 113
10 Acetone
11 Dichloromethane
12 Hexane
13 Ethyl acetate
14 Tetrachloromethane
15 Benzene
16 Methylcyclohexane
17 Toluene
18 Hexanal
19 Tetrachloroethane
20 Ethylcyclohexane
21 Ethylbenzene
22 *o*-/*p*-Xylene
23 Styrene
24 α-Pinene
25 Decane
26 Trimethylbenzene
27 Limonene
28 Undecane
29 Benzyl alcohol
30 Nonanal
31 Dodecane
32 Tridecane
33 Tetradecane

Pumped sampling can capitalise on Markes' backflush technology, by enabling tubes and traps to be packed with multiple beds of sorbent with different strengths. This allows analytes over a wide volatility range to be collected in a single run.

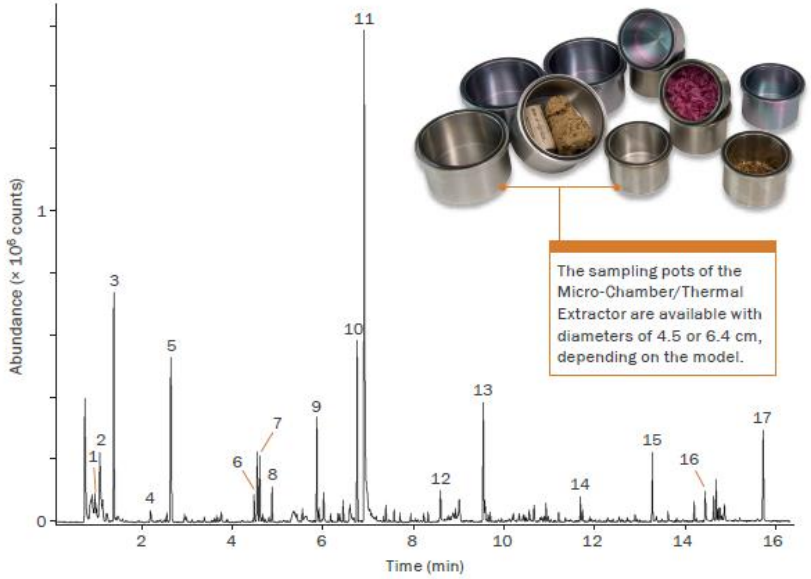


- Indoor pollutants typically arise from sources such as:
  - construction materials,
  - furnishings,
  - cleaning products
  - and consumer goods,
  - As well as activities such as cooking and smoking

A wide range of potentially harmful chemicals at ppt and ppb levels are identified in this indoor air sample, collected by pumped sampling onto sorbent tubes over relatively short time periods.

Indoor air quality

Assessing the cause of poor indoor air quality



- To more accurately assess the source materials can be put into chambers to rate the emissions.
- As part of EU regulations products used in the constructions of homes must VOCs below a set threshold to ensure indoor air concentrations do not become harmful to those residing in them.

Reflecting the versatility of TD, a range of VOCs and SVOCs – from butane (C_4H_{10}) to squalene ($C_{30}H_{50}$) – are identified in this headspace–TD analysis of mahogany using the Micro-Chamber/Thermal Extractor.

Breath sampling

How it works

- Alveolar (‘end-tidal’) breath collected and transferred onto sorbent tube
  - Provides information on VOC levels in blood (Pollutants and metabolites)

➢ **Markes’ Bio-VOC**

➢ **ReCIVA breath sampler**
(Owlstone Medical)

Challenges with breath sampling

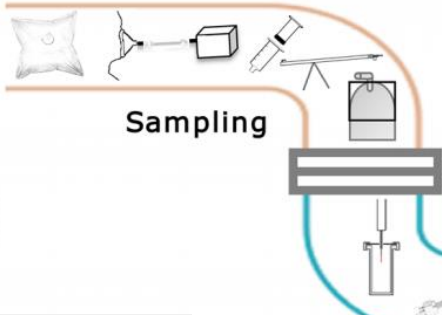
1. Compounds in breath are often at very low concentrations
   - ✓ Pre-concentration

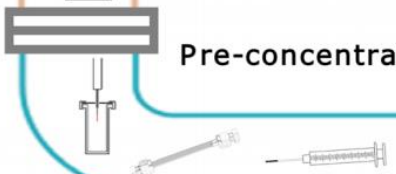
2. Breath samples can be very humid – how do we remove water without removing compounds?
   - ✓ Water management technologies – sorbent selection & dry purge

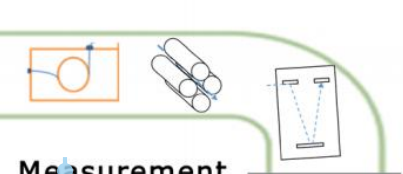
3. I need to analyse SVOCs as well as VOCs
   - ✓ Sorbent tube sampling ($C_{2/3}$ – C_{44})

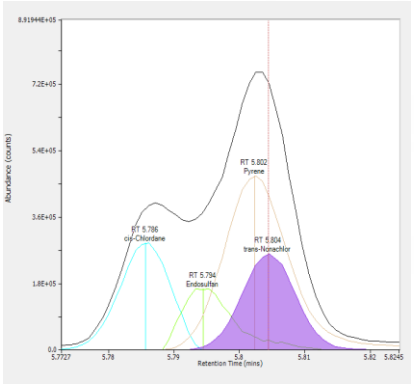
4. I need to sample at many remote locations
   - ✓ Sorbent tube sampling ($C_{2/3}$ – C_{44})

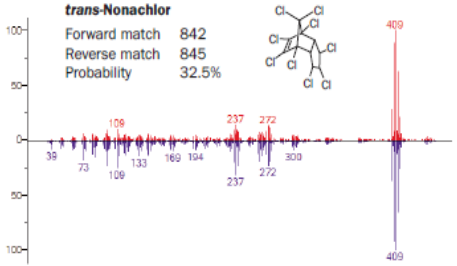
Analytical challenges in breath analysis











Source: Lawal et al., *Exhaled breath analysis: a review of 'breath-taking' methods for off-line analysis* (2017) Metabolomics, 13:110

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