Mobile Laboratory with Vocus PTR-TOF

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Mobile laboratory addresses real-world problems

Industry

Regulatory

Research
Mobile measurements are challenging

**Challenge**

- VOCs are dilute and diverse
- Accurate reporting
- Rapid measurement
- Harsh environment

**Instrument requirements**

- Extremely high sensitivity
- Wide range of measurable VOC
- Precise identification
- Semi-quantitative estimations
- Direct measurement of air up to 10 Hz
- Simultaneous measurement of all VOC
- Shock resilience
- Small, low power
- Low or no consumables
PTR-TOF technology is ideal for ambient measurement

1. Reagent ions are made in plasma source (H$_3$O$^+$)
2. Air with VOCs enters the reaction chamber
3. VOCs are ionized by the reagent
4. Ion beam is focused and air is removed
5. Ions are extracted orthogonally into TOF chamber
6. Ions are separated by mass-to-charge ratio

Time-of-flight (TOF) chamber

Number of ions vs. m/Q
PTR-TOF technology is ideal for ambient measurement

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<th>Challenge</th>
<th>Instrument requirements</th>
<th>Vocus PTR</th>
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<tr>
<td>VOCs are dilute and diverse</td>
<td>• Extremely high sensitivity</td>
<td>• Sub-ppt LOD achievable</td>
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<tr>
<td></td>
<td>• Wide range of measurable VOC</td>
<td>• Ion chemistry accesses wide range of chemical types</td>
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<td>Accurate reporting</td>
<td>• Precise identification</td>
<td>• Resolving power up to 15000</td>
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<td>• Semi-quantitative estimations</td>
<td>• Linear response to ppm levels</td>
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<td>Rapid measurement</td>
<td>• Direct measurement of air</td>
<td>• Predictable sensitivity</td>
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<td>• Simultaneous VOC measurement</td>
<td>• 50ms response time</td>
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<td>Harsh environment</td>
<td>• Shock resilience</td>
<td>• Full spectrum analysis</td>
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<td></td>
<td>• Small, low power</td>
<td>• Robust construction</td>
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<td></td>
<td>• Low or no consumables</td>
<td>• Vocus Elf: &lt;60 kg</td>
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<td>• PTR mode: &lt;$\frac{1}{2}$ L water / month</td>
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Tofwerk engineering addresses mobile challenges

Size and power

- **Vocus Scout**
  - 小精灵系列
  - < 450W

- **Vocus S(uper)**
  - < 600W

- **Vocus 2R**
  - < 600W
Tofwerk engineering addresses mobile challenges

Shock and vibration

- Acceleration measurement made during urban drive
- Shock mount systems for Vocus Elf (left) and Vocus S (right)
Tofwerk engineering addresses mobile challenges

Tilting and movement
Tofwerk engineering addresses mobile challenges

Installation possibilities

“low tech” …

…to comfy “high tech”
Software tools easily handle complex data

- Automated, real-time data processing, display, and export
- Single-click transitions between instrument states
- Broadcast results to network

Acquility TRACK

Digitizer → Transfer data from DAQ to PC → Integrate peaks → Selection of ions → Quality control → Automated

Visualization and interpretation

Combine VOC, time, and GPS data

Calibration and processing

TOF full spectrum

DAQ supplies a sample every 0.625 ns

Typically 30'000 samples
More than 8000 km (acquiring 1s data) in three months

2000 km journey across China

Continent-wide trends: mobile science on a large scale

Total VOC (measured by PTR)

* More than 8000 km (acquiring 1s data) in three months
Continent-wide trends: mobile science on a large scale

Extent and concentration of “urban bubble” can be quantified
Continent-wide trends: mobile science on a large scale

Plume of industrial emissions across China

Nitrogen-containing compound from industrial process
VOC hotspots: mobile lab on a small scale
Diversity of VOC measured with Vocus PTR

Aromatics
- Benzene
- Toluene
- Xylenes
- C9 aromatics
- C10 aromatics
- Styrene

Hydrocarbons
- Butenes
- Cyclopentadiene
- Pentenes
- Cyclohexene

Oxyaromatics
- Phenol
- Benzaldehyde

Acids
- Acetic
- Propanoic
- Butanoic
- Hexanoic
- Octanoic

Alcohols
- Methanol
- Ethanol
- Propane diol
- Butane diol
- Pentane diol

Ketones
- Acetone
- 2,3-pentane dione

Siloxanes
- D3
- D3 hydrate
- D4
- D4 hydrate
- D5

Other
- C3 amide
- C2 nitroamine
- CCl4/CFC-11
Diversity of VOC measured with Vocus PTR

Crucial:
- Large dynamic range
- Simultaneous measurement of all ions
- High resolving power OR library of VOCs

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High resolving power = accurate identification

- Peak observed at 97.045 Th = Fluorobenzene.
- Need mass resolving power >3000 to separate from 3-Furaldehyde and 2-ethyl furan.

Every digit on the mass axis matters!
Stable TOF = accurate identification

- H7O3+
- C3H7O+
- C6H7O3+
Advanced techniques: source apportionment

Complex mixture of many VOCs

Smaller number of independent sources

Each with distinct VOC composition

Matrix factorization

\[ \text{measurements} = \text{Profile 1} \times + \text{Profile 2} \times + \ldots \quad (+ \text{residual}) \]
Source apportionment of petrochemical plant

Source mixing ratios vs. drive time

Contribution of each source to total VOC

Source VOC profiles

siloxanes
Summary

Mobile laboratory addresses real-world problems

- Vocus PTR-TOF technology is ideal for mobile platforms
- Tofwerk engineering answers mobile challenges
- Software tools easily handle complex data

Examples

- Continent-wide trends: mobile science on a large scale
- VOC hotspots: mobile lab on a small scale
- VOC diversity and source apportionment
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