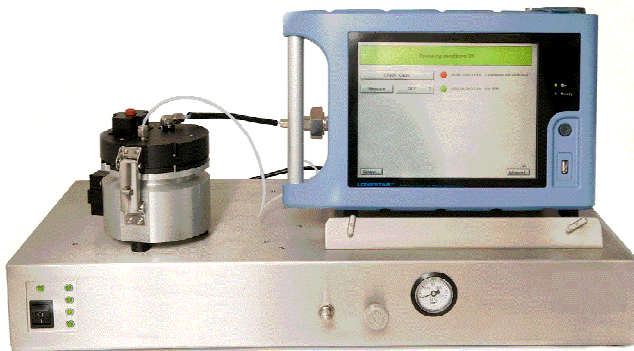


## Innovative Detection Technology

# LONESTAR™

## FIELD ASYMMETRIC ION MOBILITY SPECTROMETRY

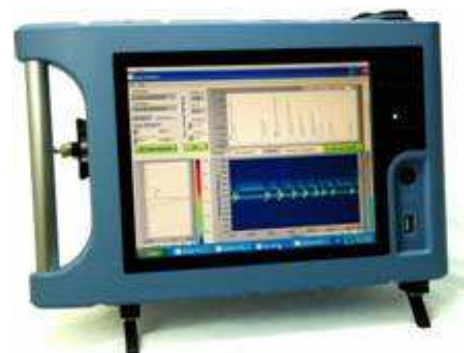


### Benefits

- Complete flexibility to „train“ instrument for a broad range of processes
- Cost-effective, easy-to-use instrument
- Reduce running costs and improve efficiency with fast analysis
- Real-time, online, granular monitoring for rapid identification of anomalous events
- Portable with a compact footprint
- Standalone operation with integrated sampling and processing
- High sensitivity with part per billion detection levels combined with inlet control for high dynamic range
- Integrated temperature, flow and humidity sensors for stable, closed-loop operation
- Network and wireless (optional) connectivity for remote monitoring and operation
- Easy integration of other sensor data and control of third party systems
- Powerful custom software for data visualization, real-time control and offline analysis

### What is it?

Lonestar is a powerful and adaptable chemical monitor in a portable, self contained unit. Incorporating Owlstone's FAIMS technology, the instrument offers the flexibility to provide both rapid alerts and detailed sample analysis. It can be trained to respond to a broad range of chemical scenarios and can be easily integrated with other sensors and third party systems to provide a complete monitoring solution. As a result, Lonestar is suitable for a broad variety of application ranging from online/ at line process monitoring to lab based R&D.



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## Applications

The Lonestar™ can be used wherever there is the need for a low power and low cost yet highly sensitive and selective method of detection. It is broadly applicable to a wide range of applications across a variety of markets.

### Defense and Homeland Security

- o Detection of explosives and chemical warfare agents – detection and identification of explosives and chemical warfare agents to protect from acts of terrorism
- o Narcotics detection – detection of concealed contraband to counter trafficking of illicit substances
- o Water contamination – detection of atypical contaminants in the water system that may pose a risk to public safety

### Industrial

- o Process monitor – monitor and optimize the operation of a process and diagnose errors by indicating a fault when the “smell” of a process line deviates from normal
- o Dangerous gas monitor – check the environment for toxic or flammable gasses that may endanger individuals, factories or equipment
- o Petrochemical gas sensor – detection of a wide variety of combustible gasses and volatile organic compounds (VOCs) in general, as well as contaminants in various hydrocarbon streams

### Automotive

- o Hydrocarbon monitor – analysis of hydrocarbons in engine exhaust for better control of engine functions to maximize performance and minimize emissions
- o Nitrogen oxides monitor – monitoring of nitrogen oxides (NO<sub>x</sub>) concentrations in exhaust gas to ensure values do not exceed permissible limits
- o Cabin air quality sensor – detection of volatile organic compound (VOCs) and other pollutants inside a car for cabin air quality management

### Environmental

- o Air quality monitor – monitor specific pollutant compounds for regulatory enforcement and cleanup efforts
- o Emissions monitor – monitor the emission of harmful industrial gasses into the atmosphere that may damage the environment
- o Detection of toxic industrial compounds – test for the release of toxic compounds, monitor decontamination efforts, and confirm effective remediation of the chemical agent
- o Water quality monitor – monitor for contamination and toxicity to ensure the safety of drinking water supplies

### Consumer

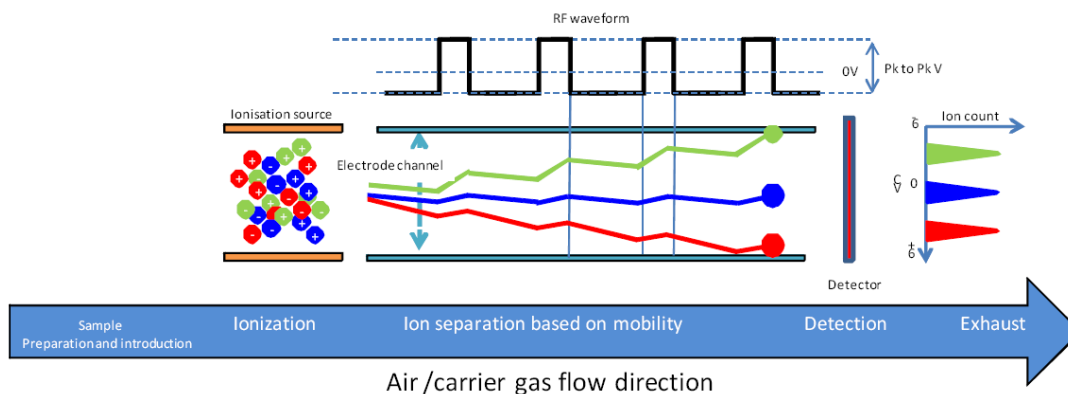
- o Advanced smoke detector – detect gases emitted prior to combustion for earlier alarm and lower false alarm rate
- o Indoor air quality monitor – general air quality monitor with the analytical capability to detect and identify major pollutants of interest

### Medical

- o Diagnostic instrument – analysis of breath or bodily fluids for non-invasive diagnostics or monitoring of treatment disease
- o Treatment monitor – analysis of breath or bodily fluids for non-invasive monitoring of treatment efficacy and progress
- o Anesthesia and respiratory monitor – detect exhaled anesthesia agents and other relevant indicators in the breath to minimize the response time of clinicians to vital signs

## Technology at a glance

Field asymmetric ion mobility spectrometry (FAIMS), also known as differential mobility spectrometry (DMS), is a gas detection technology that separates and identifies chemical ions based on their mobility under a varying electric field at atmospheric pressure. Figure 1 is a schematic illustrating the operating principles of FAIMS.



*Figure 1: FAIMS schematic. The sample in the vapor phase is introduced via a carrier gas to the ionization region, where the components are ionized via a charge transfer process or by direct ionization dependent on the ionisation source used. It is important to note that both positive and negative ions are formed. The ion cloud enters the electrode channel, where an RF waveform is applied to create a varying electric field under which the ions follow different trajectories dependent on the ions' intrinsic mobility parameter. A DC voltage (compensation voltage) is swept across the electrode channel shifting the trajectories so different ions reach the detector, which simultaneously detects both positive and negative ions. The number of ions detected is proportional to the concentration of the chemical in the sample.*

FAIMS can be used to detect volatiles in aqueous, solid and gaseous matrices and can consequently be used for a wide variety of applications. The user requirements and sample matrix for each application define the sample preparation and introduction steps required. There are a wide variety of sample preparation, extraction and processing techniques each with their own advantages and disadvantages. It is not the scope of this overview to list them all, only to highlight that the success of the chosen application will depend heavily on this critical step, which can only be defined by the user requirements.

There are two mechanisms of introducing the sample into the FAIMS unit: discrete sampling and continuous sampling. With discrete sampling, a defined volume of the sample is collected by weighing or by volumetric measurement via a syringe, or passed through an adsorbent for pre-concentration, before it is introduced into the FAIMS unit. An example of this would be attaching a sample container to the instrument containing a fixed volume of sample. Where a carrier gas (usually clean dry air) is used to transfer the sample to the ionization region. Continuous sampling is where the resultant gaseous sample is continuously purged into the FAIMS unit and either diluted by or acts as the carrier gas. For example, continuously drawing air from the top of a process vat.

The one key requirement for all the sample preparation and introduction techniques is the ability to reproducibly generate and introduce a headspace (vapor) concentration of the target analytes that exceeds the lower limits of detection of the FAIMS device.

## Carrier Gas

The requirement for a flow of air through the system is twofold: Firstly to drive the ions through the electrode channel to the detector plate and secondly, to initiate the ionization process necessary for detection.

As exhibited in *Error! Reference source not found.*, the transmission factor (proportion of ions that made it to the detector) increases with increasing flow. The higher the transmission factor, the higher the sensitivity. Higher flow also results in a larger full width half maximum (FWHM) of the peaks, however, decreasing the resolution of FAIMS unit (see Figure 2 and Figure 3).

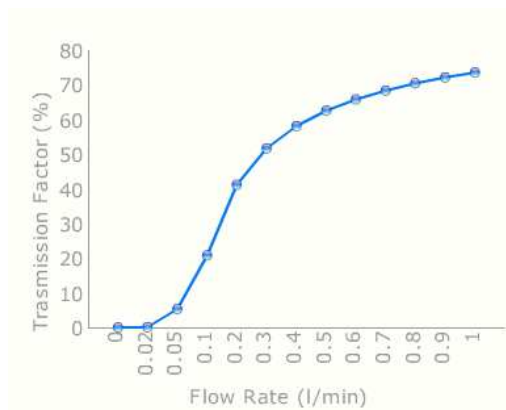


Figure2: Flow rate vs. ion transmission factor

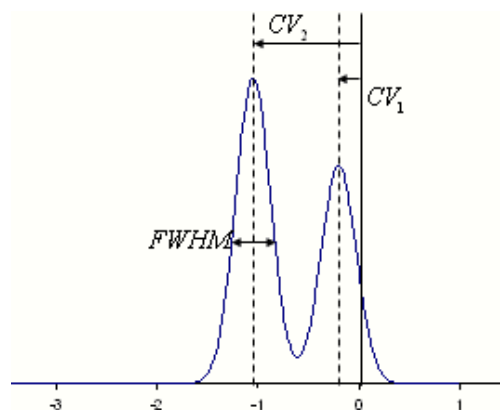


Figure3: FWHM of ion species at set CV

As the air carrier gas determines the baseline reading out the instrument. Therefore, for optimal operation it is desirable for the carrier to be free of all impurities (<0.1 ppm methane) and the humidity to be kept constant. It can be supplied either from a pump or compressor, allowing for negative and positive pressure operating modes.

## Ionization Source

There are three main vapor phase ion sources in use for atmospheric pressure ionization: radioactive nickel-63 (Ni-63), corona discharge (CD) and ultra-violet radiation (UV). A comparison of ionization sources is presented in the Table 1.

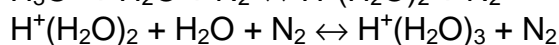
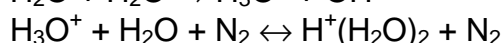
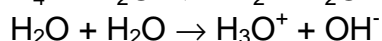
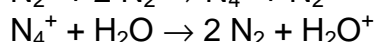
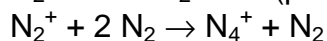
Ionisation Source	Mechanism	Chemical Selectivity
Ni <sup>63</sup> (beta emitter) creates a positive / negative RIP	Charge transfer	Proton / electron affinity
UV (Photons)	Direct ionisation	First ionisation potential
Corona discharge (plasma) creates a positive / negative RIP	Charge transfer	Proton / electron affinity

Table 1: FAIMS ionization source comparison

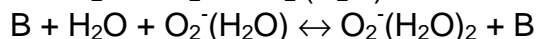
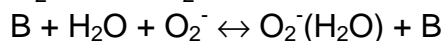
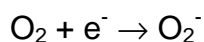
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Ni-63 undergoes beta decay, generating energetic electrons, where as CD ionization strips electrons from the surface of a metallic structure under the influence of a strong electric field. The electrons generated interact with the carrier gas (air) to form stable intermediate ions called reactive ion peak (RIP) with positive and negative charges. These RIP ions then transfer their charge to neutral molecules through collisions thus both Ni-63 and CD are known as indirect ionization methods.

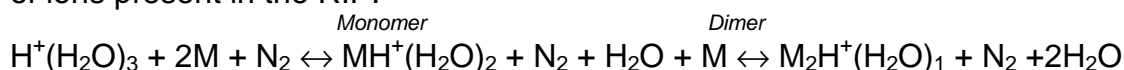
For the positive ion formation:



For the negative ion formation:



The water based clusters (hydronium ions) in the positive mode (blue) and hydrated oxygen ions in the negative mode (red), are stable ions which form the RIPs. When an analyte (M) enters the RIP ion cloud, it can replace one or (dependent on the analyte) two water molecules to form a monomer ion or dimer ion respectively, reducing the number of ions present in the RIP.



Dimer ion formation is dependent on the analyte's affinity to charge and its concentration. This is illustrated in the Figure 4 using dimethyl methylphosphonate (DMMP). In plot A it shows that the RIP decreases with an increase in DMMP concentration as more of the charge is transferred over to the DMMP. In addition the monomer ion decreases as dimer formation becomes more favourable at the higher concentrations. This is shown more clearly in plot B, which plots the peak ion current of both the monomer and dimer at different concentration levels.

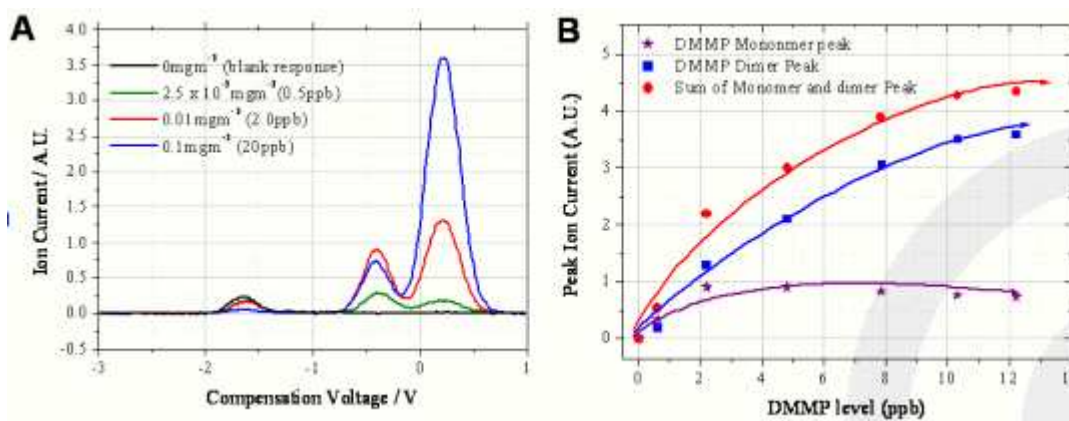


Figure 4 A+ B: DMMP Monomer and dimer formation at different concentrations

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Under the action of the indirect ionization process is the manner in which ions are formed is exactly the same, however, the likelihood of ionization is governed by its affinity towards proton and electrons (Table 2 and Table 3).

In complex mixtures where more than one chemical is present, competition for the available charge occurs resulting in preferential ionization of the compounds within the sample. Thus the chemicals with high proton or electron affinities will ionize more readily than those with a low proton or electron affinity. Therefore the concentration of water within the ionization region will have a direct effect on certain analytes whose proton / electron affinities are lower.

Chemical Family	Example	Proton affinity
Aromatic Amines	Pyridine	930 kJ/mole
Amines	Methyl amine	899 kJ/mole
Phosphorous Compounds	TEP	891 kJ/mole
Sulfoxides	DMS	884 kJ/mole
Ketones	2-pentanone	832 kJ/mole
Esters	Methyl Acetate	822 kJ/mole
Alkenes	1-Hexene	805 kJ/mole
Alcohols	Butanol	789 kJ/mole
Aromatics	Benzene	750 kJ/mole
Water		691 kJ/mole
Alkanes	Methane	544 kJ/mole

Table 2: Overview of the proton affinity of different chemical families

Chemical Family	Electron affinity
Nitrogen Dioxide	3.91 eV
Chlorine	3.61 eV
Organomercurials	↑
Pesticides	
Nitro compounds	
Halogenated compounds	
Oxygen	0.45 eV
Aliphatic alcohols	↑
Ketones	

Table 3: Relative electron affinities of several families of compounds

The UV ionization source is a direct ionization method whereby photons are emitted at energies of 9.6, 10.2, 10.6, 11.2 and 11.8 eV and can only ionize chemical species with a first ionization potential less than the emitted energy. Important points to note are that there is no positive mode RIP present when using this ionization source and also using UV ionization is very selective for certain compounds.



## Mobility

Ions in air under an electric field will move at a constant velocity proportional to the electric field. Where the proportionality constant is known as mobility.

Referring to the Figure 5, as the ions enter the electrode channel the applied RF voltages create oscillating regions of high ( $+V_{HF}$ ) and low ( $-V_{HF}$ ) electric fields as the ions move through the channel. The difference in the ion's mobility at the high and low electric field regimes dictates the ion's trajectory through the channel. This phenomenon is referred as differential mobility.

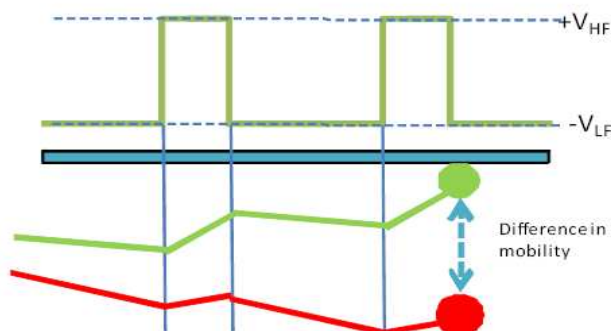


Figure5: Schematic of a FAIMS channel showing the difference in the ions' trajectories caused by their different mobilities experienced at high and low electric fields

The physical parameters of a chemical ion that affects its differential mobility are its collisional cross section and ability to form clusters within the high / low regions. The environmental factors within the electrode channel affecting the ion's differential mobility are electric field, humidity, temperature and gas density (pressure).

The electric field in the high/low regions is supplied by the applied RF voltage waveform (see Figure 6). The frequency of which relates to the number of high/low cycles per unit time. The duty cycle is the proportion of time spent within each region per cycle. Increasing the peak-to-peak voltage increases / decreases the electric field experienced in the high/low field regions and therefore influences the velocity of the ion accordingly. It is this parameter that has the greatest influence on the differential mobility experienced by the ion.

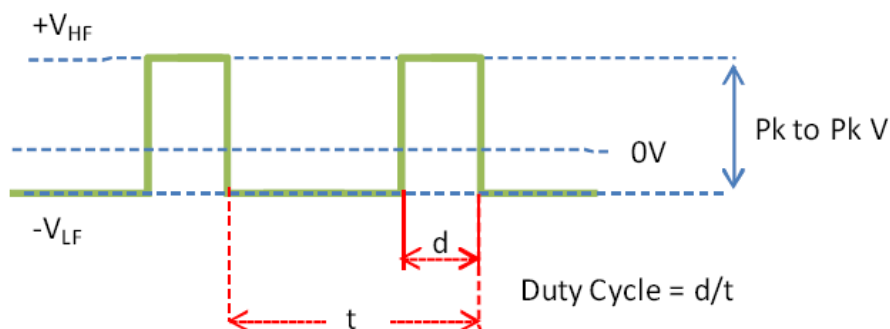


Figure6: Schematic of the ideal RF waveform, showing the duty cycle and peak to peak voltage

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It has been shown that humidity has a direct effect on the differential mobility of certain chemicals, by increasing/decreasing the collisional cross section of the ion within the respective low / high field regions. This addition and subtraction of water molecules is referred to as clustering and de-clustering. Increased humidity also increases the number of water molecules involved in a cluster ( $MH^+(H_2O)_2$ ) formed in the ionization region. When this cluster experiences the high field in between the electrodes the water molecules are forced away from the cluster reducing the size ( $MH^+$ ), this is known as de-clustering.

As the low field regime returns so do the water molecules to the cluster thus increasing the ions size (clustering) thus giving the ion a larger differential mobility.

Gas density and temperature can also affect the ion's mobility by changing the number of ion-molecule collisions and changing the stability of the clusters, influencing the amount of clustering and de-clustering.

Changes in the electrode channel's environmental parameters will change the mobility exhibited by the ions. Therefore it is advantageous to keep the gas density, temperature and humidity constant when building detection algorithms based on an ion's mobility as these factors would need to be corrected for. However, it should be kept in mind that these parameters can also be optimized to gain greater resolution of the target analyte from the background matrix, during the method development process.



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## Detection and Identification

As ions with different mobilities travel electrode channel, some will have trajectories that will result in ion annihilation against the electrodes, whereas others will pass through to hit the detector a compensation voltage (CV) is scanned between the top and bottom electrode (see Figure 7). This Process realigns the trajectories of the ions to hit the detector and enables a CV spectrum to be produced.

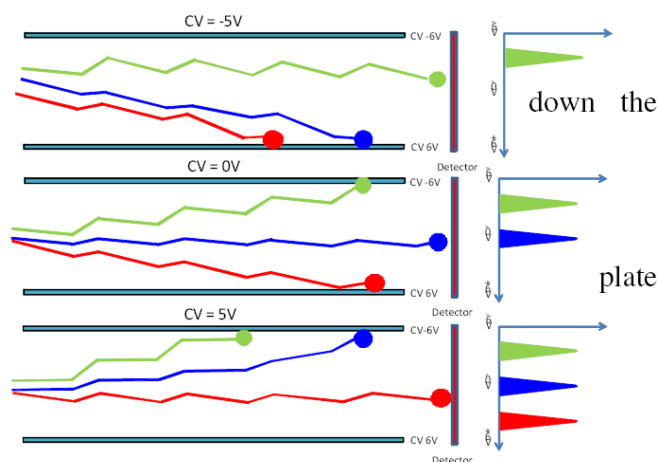


Figure 7: Schematic of the ion trajectories at different compensation voltages and the resultant FAIMS spectrum

The ion's mobility is thus expressed as a compensation voltage at a set electric field. Figure 8 shows an example CV spectrum of a complex sample where a de-convolution technique has been employed to characterize each of the compounds.

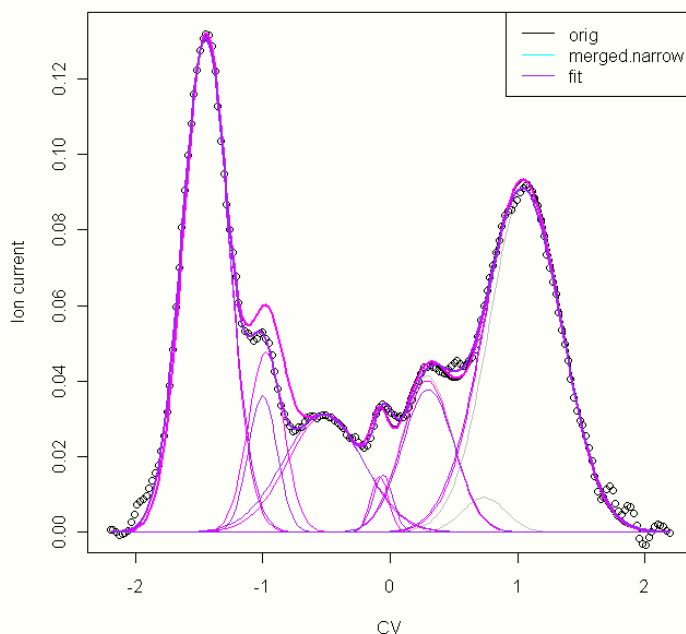


Figure 8: Example CV spectra. Six different chemical species with different mobilities are filtered through the electrode channel by scanning the CV value

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Changing the applied RF peak-to-peak voltage (electric field) has a proportional effect on the ion's mobility. If this is increased after each CV spectrum, a dispersion field matrix is constructed. Figure 9 shows two examples of how this is represented; both are negative mode dispersion field (DF) sweeps of the same chemical. The term DF is sometimes used instead of electric field. It is expressed as a percentage of the maximum peak-to-peak voltage used on the RF waveform. The plot on the left is a waterfall image where each individual CV scan is represented by compensation voltage (x-axis), ion current (y-axis) and electric field (z-axis). The plot on the right is the one that is more frequently used and is referred to as a 2D color plot. The compensation voltage and electric field are on the x, and y axes and the ion current is represented by the color contours.

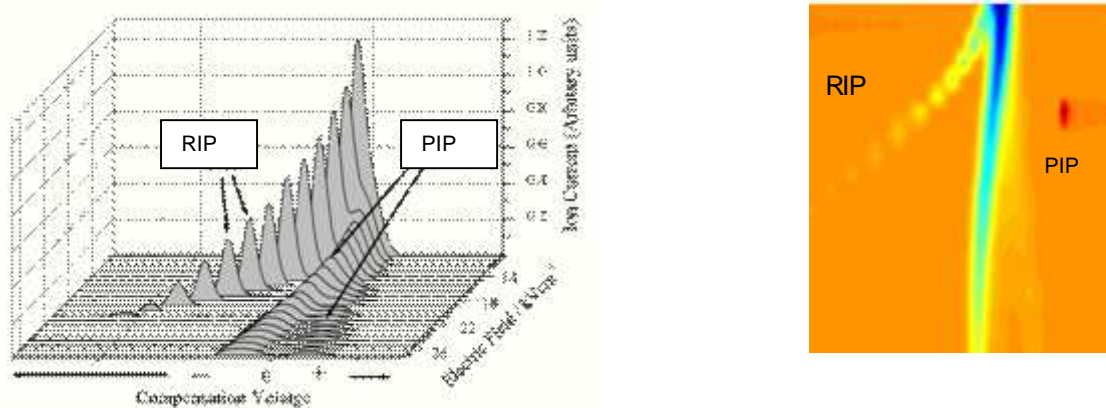


Figure 9: Two different examples of FAIMS dispersion field matrices with the same reactive ion peaks (RIP) and product ion peaks (PIP). In the waterfall plot on the left, the z axis is the ion current; this is replaced in the right, more frequently used, colorplot by color contours

With these data rich DF matrices a chemical fingerprint is formed, in which identification parameters for different chemical species can be extracted, processed and stored. Figure 10 shows one example: here the CV value at the peak maximum at each of the different electric field settings has been extracted and plotted, to be later used as a reference to identify the same chemicals.

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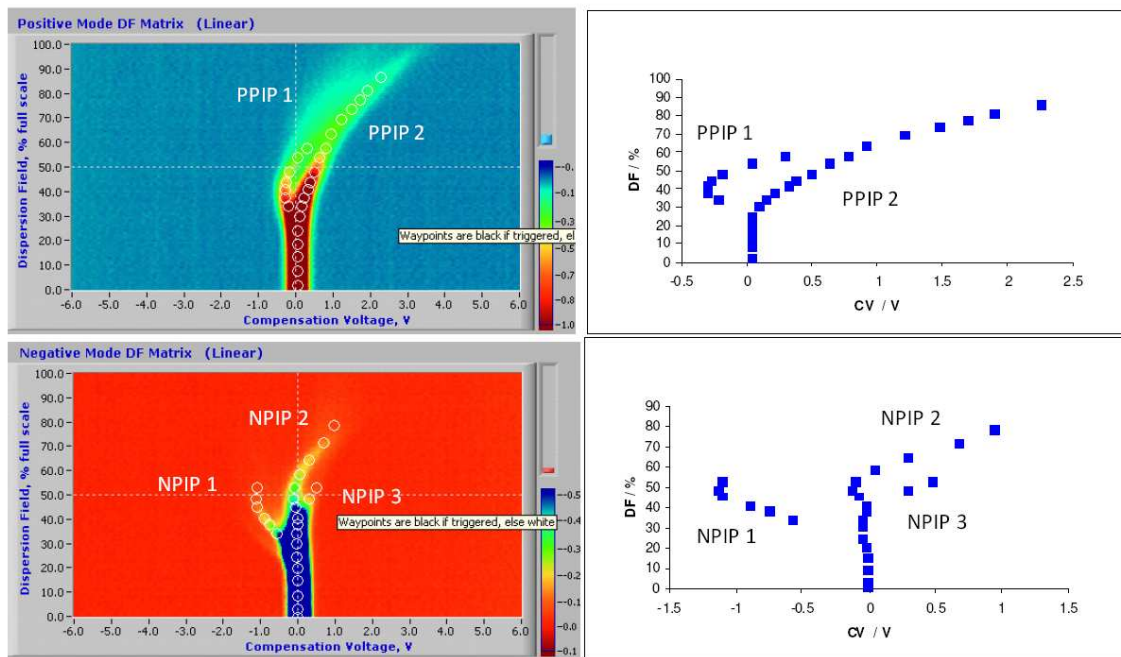


Figure 10: On the left are examples of positive (blue) and negative (red) mode DF matrices recorded at the same time while a sample was introduced into the FAIMS detector. The sample contained 5 chemical species, which showed as two positive product ion peaks (PPIP) and three negative product ion peaks (NPIP). On the right, the CV at the PIP's peak maximum is plotted against % dispersion field to be stored as a spectral reference for subsequent samples.

In Figure 11 a new sample spectrum has been compared to the reference spectrum and clear differences in both spectra can be seen.

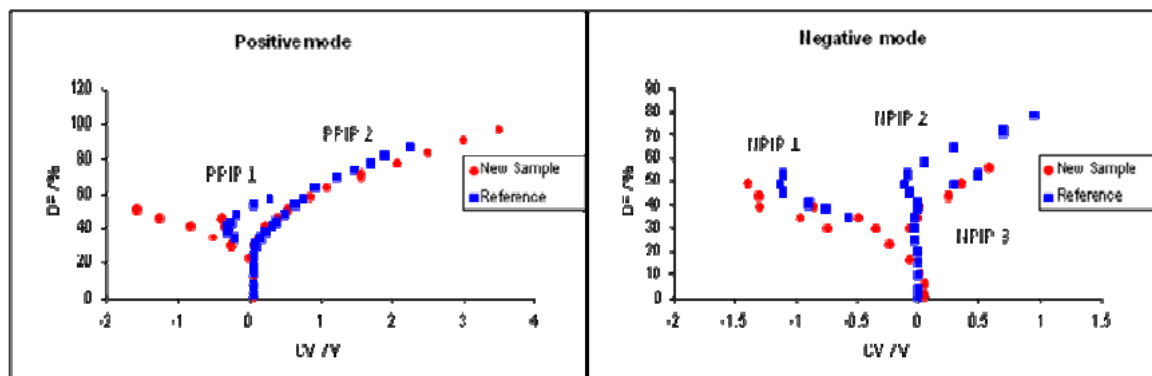


Figure 11: Comparison of two new DF plots with the reference from the Figure before. It can be seen that in both positive and negative modes there are differences between the reference product ion peaks and the new samples.

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## Technical Specification

Technology	Field Asymmetric Ion Mobility Spectrometry (FAIMS)
Detection Mode	Positive and negative ions
Sample input	Ambient, Headspace, Process line
Inlet / Outlet	1/8" Swagelok compression fittings
Analyte range	Industrial gases and VOCs
Dynamic range	User adjustable inlet dilution for ppb - % concentrations
Instrumental Air	Integrated and easy-to-replace scrubber and desiccant Connection to air line for long life, fixed point operation
Max heater temperature	70°C
Humidity Range	0% - 95 %
Instrument Sensors	Temperature, humidity, flow and pressure
Start-up time	5 minutes
Spectra analysis time	< 1sec
Inputs	Inbuilt tracker ball. Optional connectivity to keyboard and mouse
Output	Real-time chemical spectra and stored data files for offline analysis
Computer	Inbuilt PC running Windows XP
Memory	4 Gb internal storage
Comms	USB * 4. RJ45 Ethernet network connection. GPIO. Bluetooth wireless (optional)
Software	Custom online control and offline analysis software
AC Inputs	120/240 VAC
Dimensions	383 (w) x 262 (h) x 195 (d) mm
Weight	7.8 kg