



A review on ion mobility mass spectrometry

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Abstract

Mass Spectrometry can be coupled with ion mobility to get results that cannot be obtained by alone mass spectrometry. This coupled instrument can be used for knowing the separation of isomers, isobars, and conformers, the reduction of chemical noise, and the measurement of ion size. It divides ions into families of ions as well as ions with the same charge and similar structural properties. The four ion mobility separation techniques currently applied to mass spectrometry are described in this article. Low-resolution mobility separation is demonstrated by AIMS. Offering continuous ion monitorings are DMS and FAIMS. TWIMS is a novel IMS technique that has good sensitivity and is well integrated into a commercial mass spectrometer while having modest resolving power. In this review it includes that Many researches has used this technique has it gives results in millisecond and its low cost operation.it has major drawback of contamination of compounds due to atmospheric pressure, complex spectra and interferences are due to wide spread of ionization.it is not suitable for Non-volatile compound and the reproducibility is 1-2%.

Keywords: Ion mobility –mass spectrometry; DTIMS; TMS; AIMS; DMS; TWIMS

1 Introduction

From the last few years, Ion mobility spectrometry (IMS) has been a widely used scientific technique. IMS has been used to screen the identification of environmental mixtures, explosives, material fighting reagents (CWAs), and petroleum synthetic. It is founded as an independent instrument. Based on their mobilities—a ratio of a particle's size to charge—IMS isolates particles in an electric field within the sight of a latent gas. IMS can be used to separate particles before mass spectrometry and for specific particle identification following chromatographic division [1-6]. It is possible to identify the constituents, particles, and organic entities of natural or inorganic mixes. IMS is highly sensitive to organic and synthetic combat agents, explosives, and illegal drugs. IMS is used to identify these materials at customs and in airport terminals and has a wide range of uses in military applications because examination can be done extremely fast. Sample presentation, compound ionization, ion mobility division, mass partition, and particle identification are the five fundamental operations that an IMMS device should be able to carry out. Simple fume tests or the thermal desorption of semi-volatile mixtures from channels or traps are both options. Typically, fluid samples are simply injected into the IMMS [7-9].

2 Principle

The basic principle of ion mobility separation can be described as a gas-phase electrophoresis technique, whereby gaseous ions are separated according to their size, shape, and charge in the presence of neutral gas interactions within a weak electric field. The drift region is filled with an inert buffer gas (e.g., helium or nitrogen) under atmospheric pressure conditions. Depending on the specific IMS technique, ions move through the drift region either by influence of the electric field, or the flow of buffer gas. Various ions will have different mobilities in the drift region which allows the

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separation of mixtures of ions and can also provide structural information regarding the size and shape of the analytes[10-12] The simplest configuration of x electrodes are stacked along the length of the tube, and a static direct current (DC) field is applied across the electrodes, while the volume of the tube is filled with an inert buffer gas. The electric field is kept low to prevent energetically- activating the ions, and as ions move under the influence of this weakly applied electric field, their drift velocity, v_D , is subsequently governed by a combination of the electric field, E , and the gas-phase mobility of the ion, K , the latter of which is specific to the identity of the buffer gas being used[13,14].

$$v_D = KE$$

K is measured experimentally based on the time it takes an ion to traverse the drift tube of length, L .

$$K_0 = K P / P_0 T_0 / T$$

Comparisons of reduced ion mobilities, K_0 , across laboratories can be facilitated by normalizing the measurement of drift time, t_D , for buffer gas pressure, P , and temperature, T , as follows.

$$K = K_0 * (273 / T) * (P / P_0)$$

It is often useful to deduce information about the structure (i.e. the size and shape) of specific ions based on a mobility experiment. This is possible using an experimentally derived collision cross section, CCS, for an ion, which represents the average, 2-dimensional area of the molecule as it interacts with the buffer gas over a range of three-dimensional orientations.

In the above expression, q refers to the charge on the ion, k_B is Boltzmann's constant, m_I and m_B are the masses of the ion and buffer gas, respectively, and N is the number density of the buffer gas. While somewhat complex, the above fundamental ion mobility expression is algebraic and all of the parameters except CCS can be determined empirically, which allows for direct measurements to be made. By operating with various electric fields and drift gas conditions different IMS methods can be developed, each with their own specific advantages.

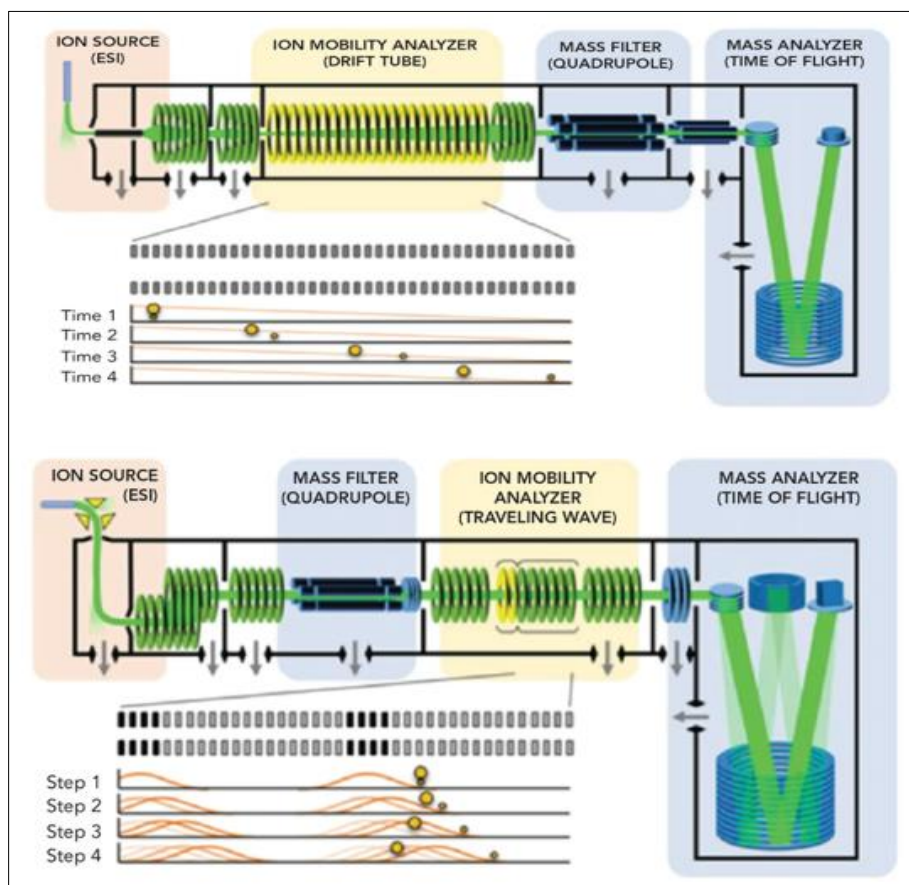


Figure 1 Working Principle of Ion mobility-Mass spectrometry

Here we discuss four common ion mobility techniques: drift tube (DTIMS), asymmetric electric field (FAIMS and DMS). In the above expression, q refers to the charge on the ion, k_B is Boltzmann's constant, m_i and m_b are the masses of the ion and buffer gas, respectively, and N is the number density of the buffer gas. While somewhat complex, the above fundamental ion mobility expression is algebraic and all of the parameters except CCS can be determined empirically, which allows for direct measurements to be made. By operating with various electric field and drift gas condition different IMS methods can be developed, each with their own specific advantage as described in fig: 1.

3 Instrumentation



Figure 2 Ion mobility-Mass spectrometry instrument

The ion mobility spectrometry consists of four basic units

- Ion source
- Ion mobility analyzers/drift tube
- Mass analyzers
- Detector

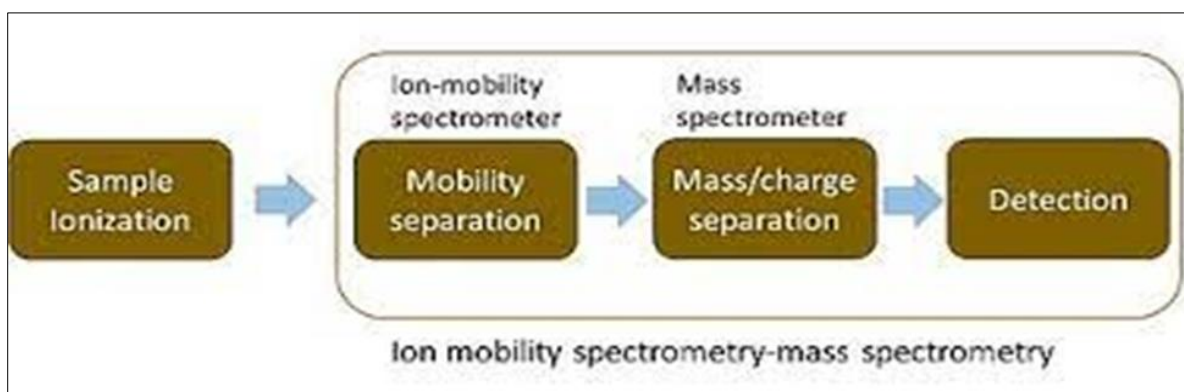


Figure 3 Block diagram of Ion mobility-Mass spectrometry

3.1 Ion Sources

^{63}Ni ionization, laser, corona spray ionization, electrospray ionization, and other sources are examples of ionization techniques used to transform molecules into ions that may be separated in the drift tube in IMS. One of them is explained in detail and others diagrams have been depicted below [15,16].

3.1.1 Electron Spray Ionisation

In the development of electron splash ionization (ESI), which Hill introduced to IMS, the range of combinations that could be dissected by IMS was greatly expanded. In the ESI interaction, a strong electric potential is supplied to the needle of the example infusion needle, creating electric charges. Electrospray occurs when the example fluid is drawn by a coulombic force from the needle toward the objective terminal that is held at a lower voltage (about 3.5 kV). As the example fluid moves toward the objective anode, soluble dissipates, passing on gradually charged beads that "detonate" due to coulombic repugnance. For fluid samples and non-unpredictable high sub-atomic weight analytes, electrospray

sources are excellent. When coupled with IMS and mass spectrometry, electrospray produces straightforward spectra without any fracture and allows for the easy resolution of the atomic weight there are different types of ionization techniques as described in fig:3,4,5.

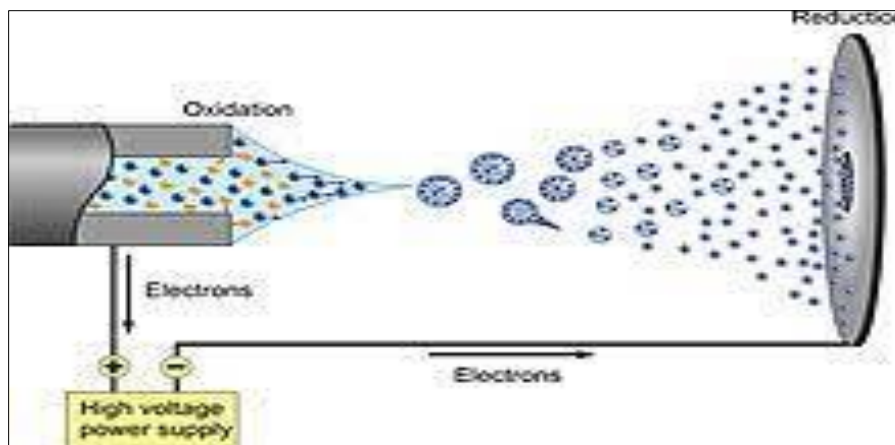


Figure 4 Electron Spray Ionization

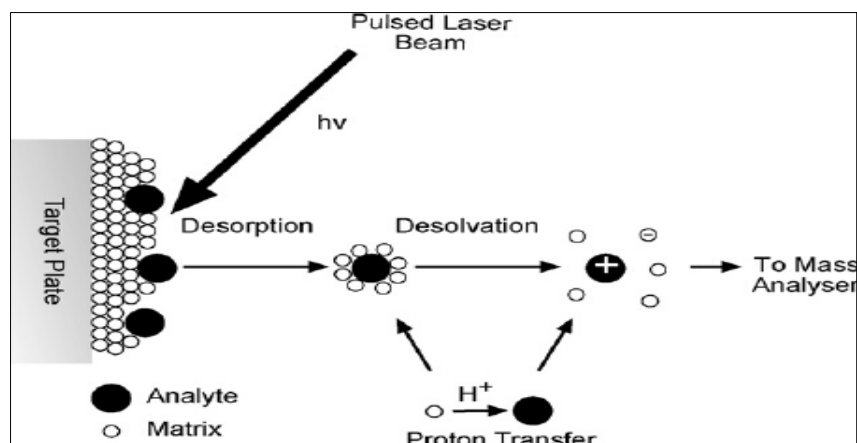


Figure 5 Matrix Assisted Laser Desorption Ionization

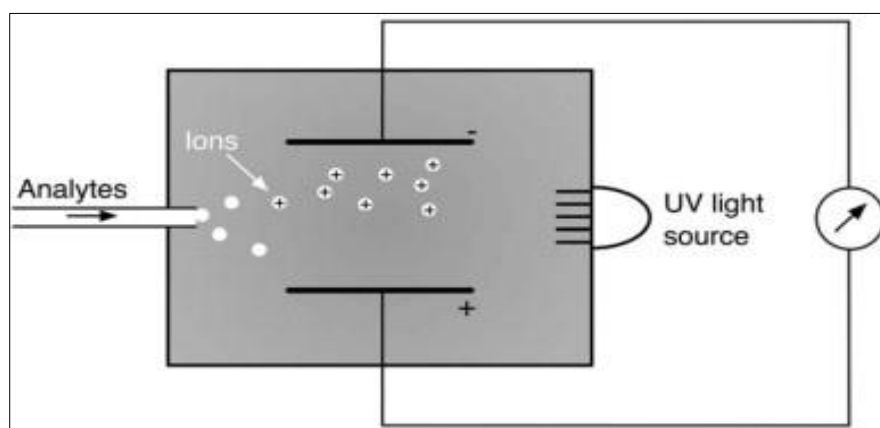


Figure 6 Photoionization

3.2 Ion mobility analyzers

Many Ion mobility analyzers are available such as Drift Tube Ion Mobility Analyzer, Travelling Wave Ion Mobility Spectrometry, Trapped Ion Mobility Spectrometry, and Differential Mass Analyzers. One is explained in detail and other diagrams are shown below.

3.2.1 Drift tube ion mobility analyzer

Typically, treated steel monitor rings are stacked between protective quartz, glass, or earthenware rings to create the float tube. In a floating time particle portability spectrometer (DTIMS), particles move through a uniform, continuous electric field in a float tube under the observation of inert gas atoms. A near, consistent electric field is created along the hub of the float tube using DTIMS, which is made up of a series of stacked-ring terminals. Drift tube particle portability spectrometry (DTIMS) is sometimes portrayed as the ideal IMS model since it offers simplicity, ease of use, and the ability to assess adaptability (and establish CCS as a crucial procedure). The consistent electric field that permeates the floating district is an essential component of DTIMS. The float region is a defined partition space where the cradle gas does not have a directed stream. Analytes move across this compressed area under the influence of a steadily provided weak electric field (often several V/cm)[17,18].

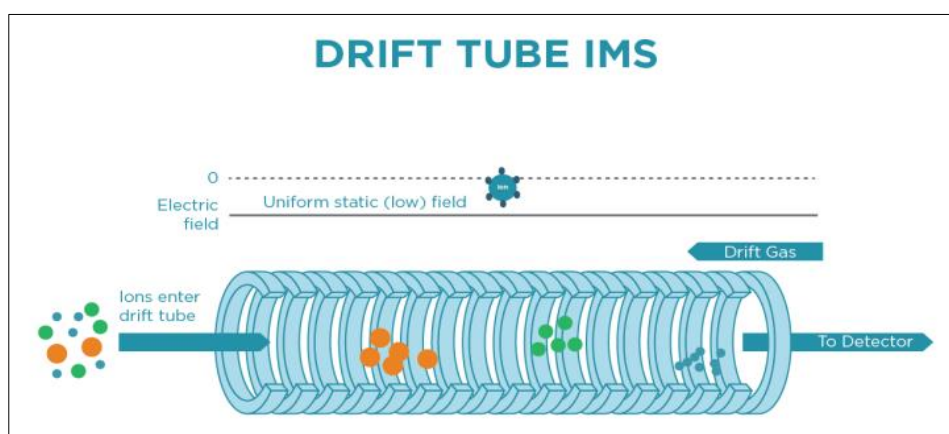


Figure 7 Drift tube IMS

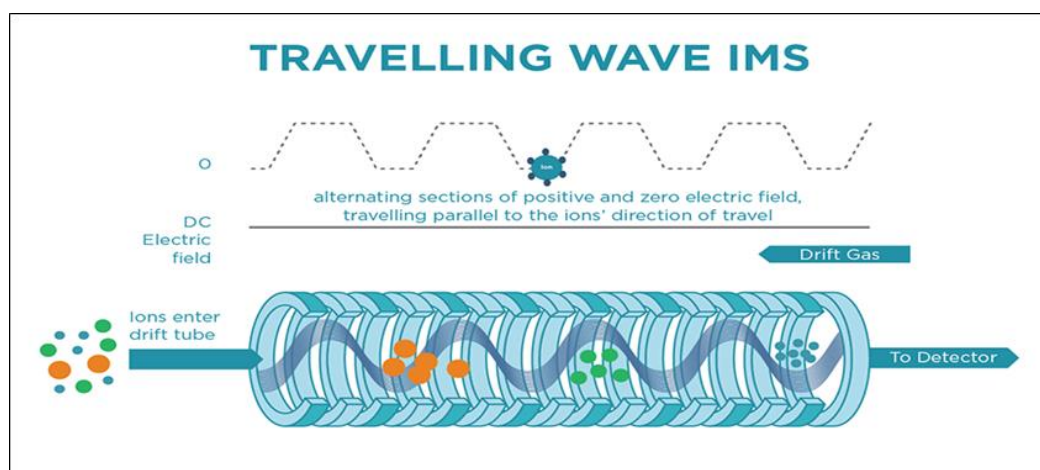


Figure 8 Travelling wave IMS

With the help of this uniform field, DTIMS is able to quantify K as a crucial technique and, in turn, determine the corresponding CCS values for analytes under the Mason-Schamp condition. In order to maintain a scientific timeline that may be combined with the chromatographic timescale, many DTIMS tests are also conducted in a CCS-aligned mode (often referred to as the single-field approach). The single-field technique has been demonstrated to provide highly reproducible CCS values, and the new paper provides additional information on it as well as several procurement strategies for DTIMS. Additionally, many commercial DTIMS devices don't require RF repression to control particle dispersion in the IMS attempt, but recent findings from Allen and Bush suggest that any tiny particle warming effects

from RF repression. How to increase the settling force of these devices is another test for DTIMS frameworks. This is accomplished by lowering the temperature and increasing the voltage drop across the float cell. Without careful centering, an expansion in either of these boundaries, however, can broaden broad pinnacles and result in particle misfortunes by creating particle dispersion. There are commercial DTIMS stages that are commonly worked at about 4 Torr and 760 Torr, respectively [19,20]. Because particle centering and achieving higher awareness is easier at lower pressures while having less of an impact on the support gas decrease separation limit, low strain frameworks are typically used. Due to difficulties in particle centering, high tension frameworks typically suffer the negative impacts of particle misfortunes at higher tensions and may not be conscious of lower pressure frameworks. There are different mass analyzers as described in figure: 5,6,7,8.

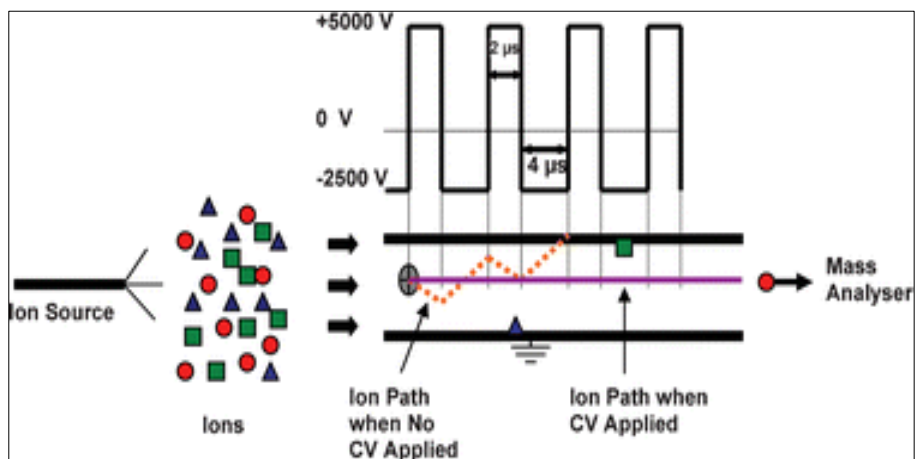


Figure 9 Tapped ion mobility mass spectrometry

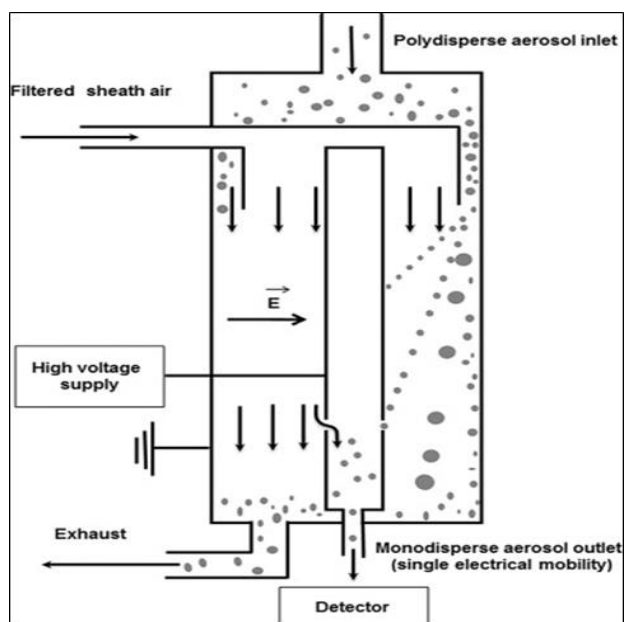


Figure 10 Differential Mass Analyzers

3.3 IMS-MS mass analyzers

- Time of Flight
- Quadrupole mass analyzer.

3.3.1 Quadrupole Mass Analyzer

Four cylindrical rods that are parallel to one another make up the structure. The quadrupole is the mass analyzer in a quadrupole mass spectrometer, which is the part of the device in charge of choosing sample ions according to their

mass-to-charge ratio (m/z). Based on the stability of their trajectories in the fluctuating electric fields that are supplied to the rods, ions are separated in a quadrupole. Four metal rods that are parallel made create the quadrupole. A radio frequency (RF) voltage with a DC offset voltage is provided between each pair of opposing rods after they have been electrically connected to one another. Ions move between the rods of the quadrupole. For a given ratio of voltages, only ions with a specific mass-to-charge ratio will enter the detector; all other ions have unstable trajectories and will strike the rods. Continually changing the applied voltage, enables the operator to select an ion with a certain m/z or to scan for a range of m/z values[21,22].

Although hyperbolic rods are preferred, cylindrical rods with a specified ratio of rod diameter to spacing offer an appropriate approximation to hyperbolas that is easier to fabricate. Resolution and peak shape are greatly affected by even small changes in the ratio. In order to fine-tune operational characteristics in light of anticipated application requirements, several manufacturers make somewhat varied ratio choices.

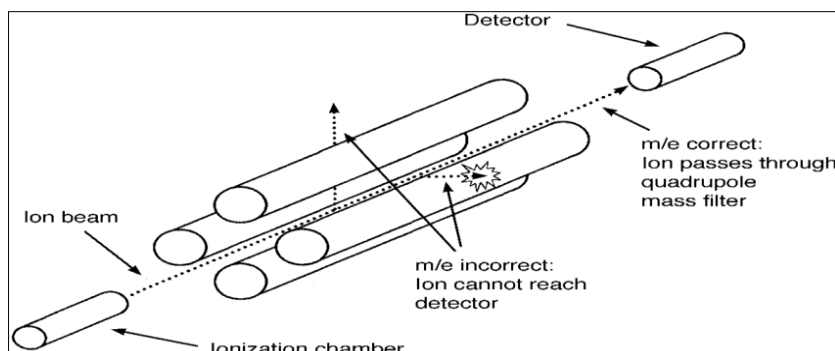


Figure 11 Quadrupole Mass analyser

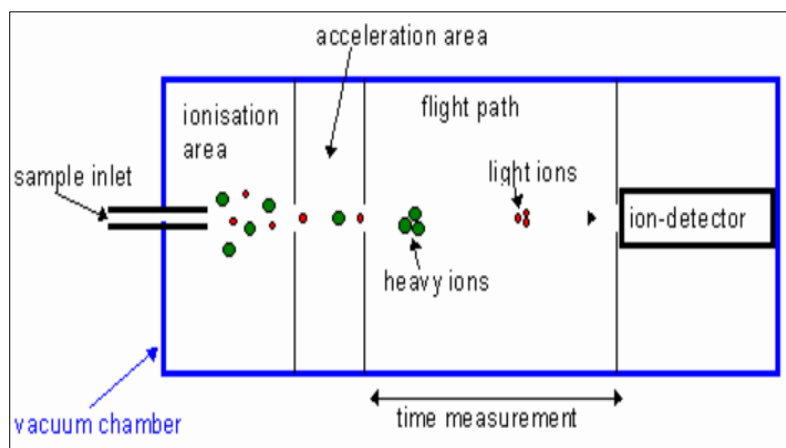


Figure 12 Time of flight

3.4 Detectors

3.4.1 Faraday Cup Detector

A metal cup is used in the experiment to collect charged particles in a vacuum. You can determine how many particles or electrons struck the cup by estimating the ensuing current. Michael Faraday, who first proposed particles in 1830, is honored by having his name attached to the Faraday cup. When a bar or bundle of particles strikes the metal, the metal gains a small net charge and the particles are destroyed. Once freed, the metal can be used to measure a small current equivalent to the number of impinging particles. The Faraday cup serves as the connecting point to the strong metal where electrons act as the charge transporters in a circuit and particles act as the charge transporters in a vacuum (as in many circuits). The number of charges being carried by the particles in the vacuum component of the circuit can be partially determined by calculating the electric flow (the number of electrons traveling through the circuit per second) in the metal piece of the circuit. The total number of particles hitting the cup in one second for unbroken light emission (each with a single charge).

$$\frac{n}{t} = \frac{I}{e}$$

Where I is the measured current (in amperes), e is the elementary charge (about 1.60×10^{-19} C), and N is the number of ions seen in time t (in seconds). As a result, one nanoamp (10^{-9} A) of measured current is equivalent to around 6 billion ions impacting the Faraday cup every second.

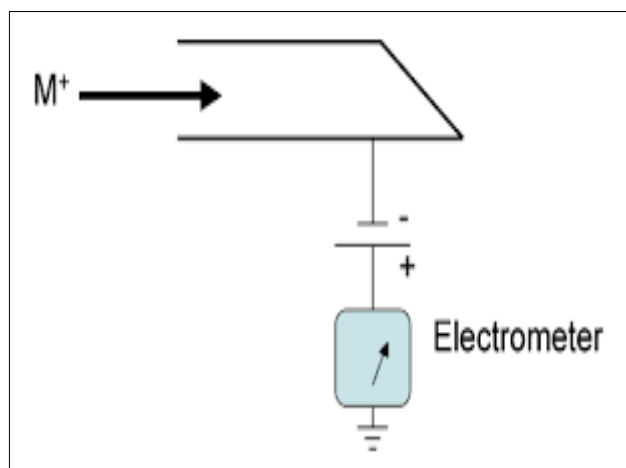


Figure 13 Faraday cup detector

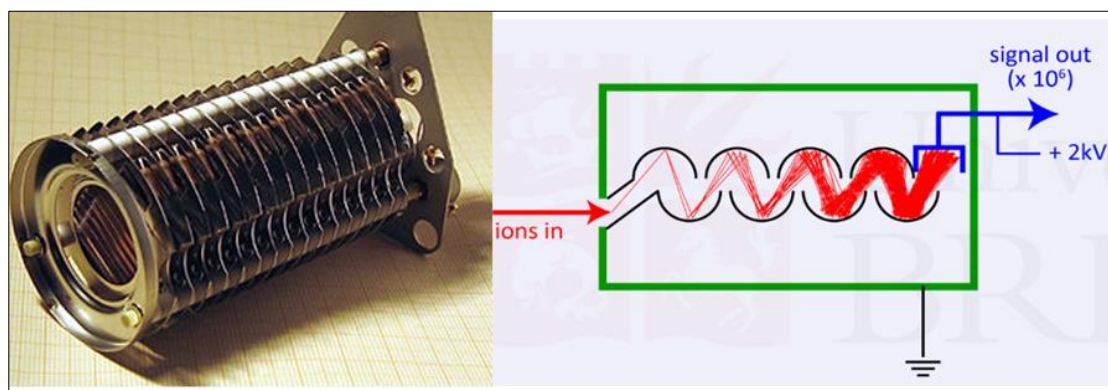


Figure 14 Electron multiplier

4 Applications

- IMS has also been used to quickly detect some types of microorganisms and poisons. It has also been used to detect various medication residues or traces of dangerous substances in a variety of food products.
- Ion Mobility Spectrometry and Its Applications in Chemical Warfare Agent Detection.
- It is utilized to separate and identify different species of isomers in a complicated combination.
- It is used in agriculture to determine the level of soil pollution. IMS is used in the detection of toxic chemicals. Various toxic chemicals (pesticides, herbicides) are used for controlling weeds, insects, and diseases in plants all over the world.
- One of the primary uses of GC-IMS in food flavor analysis is to examine sample differences. In order to do a qualitative examination of a particular VOC, GC-IMS can immediately provide the chromatographic and spectral response signals of each VOC and compare the spectral library.
- In the last ten years, ion mobility spectrometry (IMS) and related technologies have found applications in the field of food omics.

- The detection of narcotics in patients' breath, the measurement of methanol and ethanol in human saliva, and the use of volatile metabolites to identify chronic obstructive pulmonary disease are examples of applications in medicine. IMS portability and easy operation make it an essential tool for military, police, and security personnel.
- To identify volatile organic chemicals (VOCs) released from human urine, IMS was utilized in conjunction with a radioactive ionization source and a multi-capillary column.

Table 1 Case studies of IMMS

S.no	Research Done	Journal name	Conclusion	References.
1.	Ion Mobility Spectrometry: A Tool in the Forensic Science for the PostDetonation Residue Analysis	Journal of Forensic Science & Criminology	In forensic sciences the IMS methodology is mainly used as a detection device to prove the presence of latent traces of illicit drugs or explosives on surfaces of suspicious or confiscated material of evidence. IMS has successfully been used for many years to detect traces of explosives at airports and other securityCheck points; illicit drugs in prisons, cargo, and in border security. The military have long used IMS for detection of chemical warfareagents.	[13-19]
2.	IMS was used for the determination of endogenous and exogenous compounds in biological matrices such as plasma, urine, saliva, sweat, infected tissues, infected exudates, feces, breath, and breast milk are under continuous development as a consequence of society's growing interest in improving the knowledge of individuals' health conditions.	MDPI	One can realize that FAIMS or DMS are the techniques of choice when the separation of the compound of interest from other matrix components is the main objective of the analysis, as they achieve a clear improvement in the sensitivity by reducing background noise. The separation of closely related compounds such as isomers is also the main focus of space-dispersive categories.	[29-35]
3.	High Field Asymmetric Waveform Ion Mobility Spectrometry in Nontargeted Bottom-up Proteomics of Dried Blood Spots	Journal of proteomes	The results suggest that FAIMS may have a role to play in DBS proteomics by addressing the challenges of sample complexity and dynamic range.	[20-24]
4.	On-Tissue Protein Identification and Imaging by MALDI-Ion Mobility Mass Spectrometry	American Society for Mass Spectrometry.	In this article, this is illustrated with mass and time selected ion images representing specific tissue distributions for different isobaric tryptic peptides.	[25-28]

5 Conclusion

IMS is experiencing continual innovation through novel instrument developments, new methods of acquiring and filtering data, and continually developing computational strategies, all of which provide increasing confidence in mobility information acquired both experimentally. IMS-MS technology are attracting new scientists to the community

daily, and the potential applications of these analytical strategies are still being discovered. Recent developments have even interfaced IMS to ultra-high resolution mass analyzers such as the Orbitrap MS and Liquid chromatography, gas chromatography. many researches has been done as it gives fast and accurate results then other techniques separation occurs in high atmospheric pressure .it has major disadvantage it may causecontamination by high pressure and it is non-suitable for Non –volatile compounds.

Compliance with ethical standards

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Disclosure of conflict of interest

No conflict of interest.

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